Seq	Term	Variable	Description	Category1|Category2	Freq
1	&cntrl	&cntrl	A namelist in Amber input files for general simulation controls	data format|identifier	139
2	&dprc namelist	&dprc	Namelist in the Amber input file for controlling the DPRc correction	data format	4
3	&extpot namelist	&extpot	A namelist for defining the parameters of an external potential	data format	3
4	&pb namelist	&pb	A namelist in the MMPBSA.py input file for Poisson-Boltzmann parameters	data format	21
5	&rism namelist	&rism	A namelist in the MMPBSA.py input file for 3D-RISM parameters	data format	9
6	Library file	.lib	Amber file format storing residue definitions and charges.	data format	13
7	3D-RISM	3D-RISM	Three-dimensional reference interaction site model for solvation calculations	method|model	129
8	A	A	The effective electrostatic size of the molecule in the ALPB model	measure|identifier	5930
9	accept	accept	The iteration convergence criterion for the PB solver	identifier|measure	14
10	ACE (acetyl cap)	ace	An N-terminal capping group (CH3CO) for protein fragments.	chemical entity|identifier	27
11	Active site focusing	Active site focusing	A method to focus PB calculations on a specific region of interest	method	2
12	Adaptive Solvent QM/MM	vsolv=2	A QM/MM method where solvent molecules can dynamically enter the QM region	method|model	12
13	Adaptively Biased Molecular Dynamics	ABMD	A method for free energy calculation using an adaptive bias potential	method|algorithm	79
14	add12_6_4	add12_6_4	A parmed command to add C_4 terms for the 12-6-4 potential	software|process	8
15	addIons	addIons	LEaP command to add counterions around a solute using a Coulombic grid	software|method	11
16	AddToBox	AddToBox	A program to place solvent molecules into a crystal unit cell.	software	18
17	Charge Adjustment	adjust_q	Controls how charge is conserved in QM/MM simulations with link atoms	method|state	5
18	ala	ala	Input variable for the group transfer free energy of Alanine	identifier|measure	109
19	Analytical Linearized Poisson-Boltzmann	alpb	Flag to use the Analytical Linearized Poisson-Boltzmann model.	model|method	42
20	AM1	am1	A semi-empirical quantum mechanics method for charge calculation	model|method	67
21	AM1-BCC	AM1-BCC	A semi-empirical charge model combining AM1 and bond charge corrections.	method|model	20
22	amb2chm_psf_crd.py	amb2chm_psf_crd.py	A script to convert Amber prmtop/inpcrd to CHARMM psf/crd.	software	5
23	amb2gro_top_gro.py	amb2gro_top_gro.py	A script to convert Amber prmtop/inpcrd to GROMACS top/gro.	software	5
24	AMOEBA Force Field	iamoeba	A polarizable force field model.	model	10
25	Angle CV	ANGLE	Reaction coordinate defined as the angle formed by three atoms.	measure|model	232
26	Angstrom	Å	Unit of length commonly used for atomic distances	unit	219
27	antechamber (program)	antechamber	assignment.	software	88
28	Adaptive Poisson-Boltzmann Solver	APBS	A software package for solving the Poisson-Boltzmann equation	software	36
29	arad	arad	Input variable for the effective electrostatic size (A) in ALPB	identifier|measure	9
30	arcres	arcres	The resolution of dots used to represent solvent accessible arcs	identifier|measure	10
31	Adaptive String Method	ASM	Method for finding the Minimum Free Energy Path in CV space.	method|algorithm	13
32	asymmetric unit	asymmetric unit	The smallest part of a crystal structure from which the whole is generated by symmetry.	chemical entity|model	2
33	bridge function	b	A term in the closure relation representing complex many-body correlations	model|measure	279
34	bb	bb	Input variable for the group transfer free energy of the backbone	identifier|measure	6
35	bcopt	bcopt	Option for the boundary condition of the PB calculation	identifier	24
36	Bennett Acceptance Ratio	BAR	A method for calculating free energy differences between two states	method|algorithm	221
37	Berendsen Thermostat	Berendsen Thermostat	A weak-coupling algorithm for temperature control.	algorithm|method	2

38	bfgs	bfgs	OptC4.py.	algorithm|method	4
39	BiCG	BiCG	Biconjugate gradient, a solver for linear systems	algorithm	4
40	bond	bond	LEaP command to manually create a covalent bond between atoms.	software|process	396
41	buffer	buffer	The minimum distance between the solute and the edge of the RISM solvation box	measure	110
42	Buffer Region Charge	buffercharge	Total charge of the user-specified buffer atom list	measure	6
43	Buffer Region	buffermask	A region surrounding the dynamical QM region to converge forces	model	23
44	car_to_files.py	car_to_files.py	A program to generate mol2 and PDB files from a .car file.	software	5
45	CartHess2FC.py	CartHess2FC.py	A program to calculate force constants from a Cartesian Hessian matrix.	software|process	5
46	cavity_offset	cavity_offset	An offset to correct the non-polar free energy contribution in PB	measure	3
47	cestats	cestats	A program to analyze and process output from constant redox potential simulations.	software	16
48	cg	cg	Conjugate Gradient, an optimization method for parameter fitting.	algorithm|method	54
49	CHAGB	CHAGB	Charge Hydration Asymmetric Generalized Born model	model|method	14
50	CHARMM	CHARMM	A widely used molecular simulation program and its associated force fields.	software|model	128
51	charmmlipid2amber.py	charmmlipid2amber.py	A script to convert CHARMM lipid parameters to Amber format	software	5
52	ChBox	ChBox	A program to modify the box information in an Amber coordinate file.	software	5
53	closure	closure	Keyword to specify the closure approximation(s) to be used	identifier	66
54	Correction Map Energy	cmap	The correction map energy contribution for coupled torsions (CHARMM).	measure	33
55	Con2SES-3D	Con2SES-3D	A machine-learned solvent excluded surface model with high accuracy	model|software	4
56	Constant pH Molecular Dynamics	CpHMD	A method to simulate systems at a constant pH value	method|process	52
57	Core Region Charge	corecharge	Total charge of the user-specified core atom list	measure	6
58	Core QM Region	coremask	Atoms that are always treated quantum mechanically	model	16
59	cphstats	cphstats	A program to analyze and process output from constant pH simulations.	software	34
60	cpin	cpin	An input file defining protonation states for constant pH simulations.	data format	75
61	cpout	cpout	An output file containing protonation state data over a trajectory.	data format	90
62	cpptraj	cpptraj	Main trajectory analysis utility for post-processing simulations	software	50
63	CUDA	CUDA	NVIDIA's parallel computing platform and programming model for GPUs.	software	174
64	Non-bonded Cutoff	cut	Distance for truncating non-bonded interactions.	measure|unit	130
65	cutfd	cutfd	Cutoff distance for short-range finite-difference interactions	identifier|measure	8
66	cutnb	cutnb	Cutoff distance for non-bonded van der Waals and Coulombic interactions	identifier|measure	10
67	CYX	CYX	Residue name for a Cysteine involved in a disulfide bridge	chemical entity|identifier	12
68	damping function	damping function	A function used to moderate electrostatic interactions at short distances.	model|method	6
69	decompopt	decompopt	Option to select the decomposition scheme for non-polar energy	identifier	6
70	Energy Decomposition	decomposition	Specifies the type of per-residue or pairwise energy decomposition	method|process	100
71	DeePMD-kit	DeePMD-kit	A software package for training and running deep potential models	software	12
72	deleteBond	deleteBond	ParmEd command to remove a bond and associated valence terms.	software|process	6
73	Delphi	Delphi	A program for solving the Poisson-Boltzmann equation	software	18
74	DFTB 3rd Order Correction	dftb_3rd_order	Specifies third-order diagonal corrections to DFTB2	model|method	7
75	DFTB Electronic Temperature	dftb_telec	Electronic temperature in Kelvin to accelerate DFTB convergence.	measure|method	5

76	Empirical Dispersion Correction	dftb_disper	An empirical term added to correct for dispersion interactions	model|method	6
77	DFTB Max Iterations	dftb_maxiter	Maximum number of self-consistent charge (SCC) iterations for DFTB	measure	5
78	dgij	dgij	Flag to control printing of pairwise electrostatic interaction energies	identifier	2
79	Dielectric Constant	dielc	The dielectric constant of the medium.	measure|model	75
80	DIIS Attempts	ndiis_attempts	Number of DIIS extrapolation attempts to aid SCF convergence	measure	7
81	disang file	disang	An Amber input file specifying distance, angle, and dihedral restraints	data format	74
82	Dispersion Energy	disp	The dispersion energy contribution to the total energy.	measure	3
83	DPRc	DPRc	Deep Potential Range Corrected neural network correction for QM/MM potentials	model|method	16
84	DPRc activation	idprc	An integer flag to activate the DPRc machine learning correction	state	3
85	DPRc averaging	avg	A flag to use the average of multiple DPRc correction models	state	11
86	DPRc cutoff	rcut	A cutoff to dynamically select nearby atoms for the DPRc correction	measure|unit	8
87	DPRc intermolecular file	interfile	Neural network parameter file for QM/QM and QM/MM interactions	data source|data format	10
88	DPRc intramolecular file	intrafile	Neural network parameter file for QM/QM interactions only	data source|data format	6
89	DPRc mask	mask	Amber selection string for atoms to be corrected by the DPRc potential	identifier	163
90	dprob	dprob	The radius of the solvent probe used to define the molecular surface	identifier|measure	14
91	Driven ABMD	D-ABMD	A method combining SMD and ABMD for efficient pathway exploration.	method|algorithm	10
92	drms	drms	The convergence criterion for minimization based on the RMS gradient.	measure	11
93	Dynamic Lambda	dynlmb	Increment to change clambda dynamically during a simulation.	measure|process	10
94	Redox Potential REMD	E-REMD	REMD where replicas are simulated at different constant redox potentials.	method|algorithm	20
95	ECAVITY	ECAVITY	The cavity component of the non-polar solvation energy	measure|identifier	5
96	edgembar	edgembar	A program to calculate alchemical free energies using MBAR and TI	software	30
97	EDISPER	EDISPER	The dispersion component of the non-polar solvation energy	measure|identifier	2
98	EEL	EEL	The total electrostatic energy component in the output file	measure|identifier	21
99	Electrostatic Energy	elec	The electrostatic contribution to the total energy.	measure	32
100	elsize	elsize	A utility program to estimate the effective electrostatic size	software	8
101	EMAP Restraints	iemap	Restraints based on electron microscopy map data.	method|algorithm	14
102	eneopt	eneopt	Option to select the method for computing total electrostatic energy	identifier	15
103	Entropic Decomposition	entropicDecomp	Decomposes solvation free energy into energy and entropy parts	method|process	13
104	EPB	EPB	The reaction field energy component in the output file	measure|identifier	6
105	epsmem	epsmem	The dielectric constant of the implicit membrane region	identifier|measure	5
106	epsout	epsout	The dielectric constant of the exterior solvent	identifier|measure	16
107	espgen.py	espgen.py	A Python program to extract electrostatic potential from QM output.	software|process	6
108	Excess Chemical Potential	--exchem	The free energy change of adding a particle to a system	measure	28
109	FCE MTS	fcenbasis	Force-Corrected Extrapolation Multiple Time-Stepping method	algorithm|method	16
110	FEW	FEW	Free Energy Workflow, a tool for automated binding free energy calculations	software|process	159
111	FFTW	FFTW	A C library for computing the discrete Fourier transform	software	6
112	cal	fillratio	The ratio of the PB grid dimension to the solute dimension	measure	19
113	Finite-difference method	method	A numerical method for solving differential equations like the PB equation	method|algorithm	1

114	frcmod file	frcmod	An Amber file containing force field parameter modifications	data format	138
115	frcopt	frcopt	Option to compute and output electrostatic forces	identifier	10
116	Free Energy Perturbation	FEP	A method to calculate free energy differences from potential energy differences.	method|process	12
117	fscale	fscale	Ratio of coarse to fine grid spacings in an electrostatic focusing calculation	identifier|measure	4
118	gaff2	gaff2	General Amber Force Field (version 2) for organic molecules	model	18
119	Dynamics	GaMD	Enhanced sampling method adding a harmonic boost potential.	method|algorithm	76
120	Generalized Born Energy	gb	Polar solvation free energy from Generalized Born calculations.	measure	275
121	GBION	GBION	Implicit Solvent with Explicit Ions model extending the GB model	model|method	18
122	GBNSR6	GBNSR6	A Generalized Born model with numerically computed effective Born radii	model|method	22
123	gbsa	gbsa	Option to enable Generalized Born/Surface Area (GB/SA) calculations	identifier	51
124	gem.pmemd	gem.pmemd	An executable in Amber for running AMOEBA and experimental GEM* simulations	software	17
125	Generalized Born	GB1	Implicit solvent model for solvation free energy calculations	model|method	77
126	Generalized Born	GB2	Implicit solvent model for solvation free energy calculations	model|method	74
127	Generalized Born	GB5	Implicit solvent model for solvation free energy calculations	model|method	74
128	Generalized Born	GB6	Implicit solvent model for solvation free energy calculations	model|method	74
129	Generalized Born Model	generalized Born	An implicit solvent model for calculating solvation effects	model|method	73
130	GENIUSES	GENIUSES	A specific, fast machine-learned solvent excluded surface model	model|software	15
131	gi_coef_1_p	gi_coef_1_p	GBION parameter for K_GB between solute atoms and cations	identifier|measure	2
132	GTFE model	GTFE model	Group Transfer Free Energy model for pressure/temperature/osmolyte effects	model|method	0
133	H-REMD with different mdins	HAMILTONIAN	Identifier for H-REMD where replicas have different mdin parameters.	identifier|method	136
134	Hamiltonian REMD	H-REMD	REMD where replicas are simulated with different Hamiltonians.	method|algorithm	29
135	harmonic improper torsion	harmonic improper torsion	A potential term to maintain planarity using a harmonic function.	model	1
136	HIP	HIP	A special residue name for doubly protonated, titratable histidine	chemical entity	41
137	Hydrogen Mass Repartitioning (HMR)	HMassRepartition	A technique to increase hydrogen mass to allow longer timesteps	method|process	8
138	hypernetted-chain approximation (HNC)	HNC	A closure relation where the bridge function is set to zero	model|method	47
139	ibelly	ibelly	sander flag for 'belly' dynamics where only a subset of atoms move.	identifier	12
140	idecomp	idecomp	sander flag to perform per-residue or pairwise energy decomposition.	identifier	17
141	QM/MM Calculation Flag	ifqnt	Flag to enable Quantum Mechanics/Molecular Mechanics (QM/MM) calculations.	method|process	38
142	igb	igb	sander flag to enable a Generalized Born implicit solvent model.	identifier	128
143	imin	imin	sander variable to control minimization or dynamics mode.	identifier	49
144	Immersed Interface method	method (IIM)	A numerical method for solving PDEs with interfaces	method|algorithm	1
145	impose	impose	LEaP command to set internal coordinates (bonds, angles, torsions)	software	69
146	InChI-Code	InChi-Code	IUPAC International Chemical Identifier, a standard for representing molecules.	identifier	1
147	inp	inp	Option to select the method for computing non-polar solvation energy	identifier	119
148	Coordinate File	inpcrd	An Amber file format for atomic coordinates	data format	192
149	Internal Dielectric Constant	intdiel	Dielectric constant of the solute interior.	model|measure	19
150	intdiel_ion_1_p	intdiel_ion_1_p	GBION parameter for K_epsilon for solute-cation interactions	identifier|measure	3
151	Poisson-Boltzmann Solver	ipb	Flag to select the Poisson-Boltzmann solver model.	model|method	45

152	IPolQ	IPolQ	Iterative Polarizable Charge method for deriving condensed-phase charges	method|model	17
153	iprob	iprob	The radius of the mobile ion probe used to define the Stern layer	identifier|measure	4
154	Isotropic Periodic Sum	IPS	A method for calculating long-range interactions using isotropic periodic images.	algorithm|method	49
155	irest	irest	sander flag to indicate a simulation restart.	identifier	38
156	irism	irism	sander flag to enable the 3D-RISM molecular solvation method.	identifier	8
157	Max SCF Iterations	itrmax	Maximum number of iterations for the SCF procedure	measure	9
158	K_epsilon(a,b)	K_epsilon(a,b)	Coefficient scaling the electrostatic energy in the GBION model	identifier|measure	0
159	K_GB(a,b)	K_GB(a,b)	Coefficient tuning interaction energy between different atom types in GBION	identifier|measure	0
160	kcal/mol	kcal/mol	Unit of energy commonly used in molecular simulations	unit	119
161	Kernel Modified Molecular Dynamics	KMMD	A machine learning method to add corrections to a classical force field	method|algorithm|model	41
162	Kovalenko-Hirata (KH)	KH	A hybrid closure relation combining HNC and the mean spherical approximation	model|method	33
163	LEaP	tleap	A program for preparing Amber molecular mechanics input files	software	313
164	leaprc	leaprc	A script file executed at the start of a LEaP session to load standard parameters	data format|data source	110
165	GLYCAM force field	leaprc.GLYCAM_06j-1	A force field specifically parameterized for carbohydrates	model|data source	13
166	Lennard-Jones Potential	Lennard-Jones	A potential describing van der Waals forces between atoms	model	60
167	Linear Interaction Energy	LIE	A method for estimating binding free energies from interaction energies	method|model	60
168	ligand_mask	ligand_mask	An Amber mask specifying the ligand residues in the complex	identifier	7
169	Link Atom Atomic Number	lnk_atomic_no	The atomic number of the element used as a link atom.	identifier|chemical entity	2
170	Link Atom Distance	lnk_dis	Specifies the distance from a QM atom to its corresponding link atom	measure|unit	6
171	lipid21	lipid21	Recommended lipid force field for membrane simulations	model	31
172	lj1264	lj1264	sander flag to enable the 12-6-4 Lennard-Jones potential.	identifier	8
173	Low-Mode Conformational Search	LMOD	Conformational search method based on eigenvector following of low-frequency modes.	method|algorithm	102
174	loadAmberParams	loadAmberParams	LEaP command to load an AMBER parameter set file	software	13
175	loadamberprep	loadamberprep	LEaP command to load an Amber prep file.	software|process	7
176	loadMol2	loadMol2	LEaP command to load a molecule from a mol2 file.	software|process	6
177	Locally Enhanced Sampling	LES	An enhanced sampling method focusing computational effort on a subregion.	method|algorithm	161
178	makeANG_RST	makeANG_RST	A program that converts torsion angle constraints into Amber RST format	software	7
179	makeCHIR_RST	makeCHIR_RST	A program that creates chirality and omega constraints for refinement	software	6
180	makeDIST_RST	makeDIST_RST	A program that converts simplified distance bounds into sander input	software	14
181	maxcyc	maxcyc	The maximum number of minimization cycles to perform.	identifier	27
182	maxitn	maxitn	The maximum number of iterations for the PB solver	identifier|measure	15
183	maxsph	maxsph	The approximate number of dots representing the maximal atomic SASA	identifier|measure	3
184	mbondi2 radii	mbondi2	A modified set of Bondi radii for implicit solvent calculations	data source|model	15
185	mbondi3	mbondi3	A specific set of modified Bondi radii for the igb=8 GB model	data source|model	13
186	mctrdz	mctrdz	The center of the implicit membrane in the z-direction	identifier|measure	7
187	mdgx	mdgx	A program for molecular dynamics algorithm development and parameter fitting.	software	88
188	MDIIS	--mdiis_del	Modified Direct Inversion in the Iterative Subspace solver method	algorithm	29
189	mdin	mdin	The primary input file for sander, containing control parameters.	data format	224

190	mdout	mdout	The primary human-readable output file from a sander run.	data format	115
191	mdout_analyzer.py	mdout_analyzer.py	A Python script to rapidly parse and analyze energy components from mdout files	software	4
192	Mechanical Embedding	qmmm_int=0	A QM/MM coupling scheme using classical interactions between regions	method|model	16
193	membraneopt	membraneopt	Option to enable the implicit membrane model	identifier	8
194	metalpdb2mol2.py	metalpdb2mol2.py	A program to convert PDB files of metal ions into mol2 format.	software	5
195	Minimum Free Energy Path	MFEP	The most probable transition pathway between two energy minima	model|state	15
196	MLSES	MLSES	Machine-Learned Solvent Excluded Surface model	model|method	15
197	mlses_opt	mlses_opt	Option to select the runtime for the MLSES model	identifier	4
198	MMPBSA.py	MMPBSA.py	A Python script to perform MM/PB(GB)SA binding free energy calculations	software|method	71
199	mol2	mol2	A molecular file format for representing chemical structures	data format	93
200	mol2rtf.py	mol2rtf.py	A program to generate a CHARMM RTF file from a mol2 file.	software	6
201	mol3 file	mol3	A file format similar to mol2 but containing additional connectivity records.	data format	5
202	Molecular Dynamics	imin=0	Simulation method that computes the time evolution of particles	method|process	168
203	Molecular Reconstruction	--molReconstruct	Calculates molecular properties from atomic distribution functions	method|process	6
204	molsurf	molsurf	A flag to use the molsurf algorithm for surface area calculation	identifier|algorithm	10
205	MOPAC	MOPAC	A general-purpose semi-empirical quantum mechanics software package	software	9
206	mprob	mprob	The probe radius for the implicit membrane	identifier|measure	3
207	MRC 2014 format	MRC	A binary format for volumetric data, used by MRC and CCP4	data format	17
208	mthick	mthick	The thickness of the implicit membrane slab	identifier|measure	8
209	multipmemd	multipmemd	A capability in pmemd to run multiple, coupled simulations simultaneously.	software|process	13
210	multisander	multisander	A feature of sander.MPI to run multiple independent simulations simultaneously.	software|process	38
211	Multistate Bennett Acceptance Ratio	MBAR	A statistical method for calculating free energy differences from multiple states.	method|algorithm	40
212	Number of Structures CV	N_OF_STRUCTURES	conformations.	measure|model	3
213	nbuffer	nbuffer	Distance of the FD grid boundary from the solute surface	identifier|measure	3
214	ndfes	ndfes	A program to calculate free energy surfaces from umbrella sampling simulations	software	100
215	Nudged Elastic Band	NEB	Method for finding minimum energy paths between two conformations.	method|algorithm	50
216	nef_to_RST	nef_to_RST	A script to convert NMR Exchange Format (NEF) files to Amber RST format	software	4
217	NetCDF Trajectory Format	netCDF	A binary file format for storing trajectory data efficiently.	data format	61
218	Neural network atom type	mBr	Identifiers for atoms used by the neural network model	identifier|chemical entity	2
219	nfocus	nfocus	Number of focusing steps in a multi-grid PB calculation	identifier	13
220	NME (N-methylamide cap)	nme	A C-terminal capping group (CH3NH) for protein fragments.	chemical entity|identifier	29
221	nmropt	nmropt	Flag to enable distance and angle restraints in a simulation	identifier	24
222	NOE Violation Energy	noe	The energy penalty for Nuclear Overhauser Effect (NOE) violations.	measure	8
223	npbgrid	npbgrid	Frequency (in steps) for regenerating the finite-difference grid	identifier	4
224	npbopt	npbopt	Option to select between the linear or full nonlinear PB equation	identifier	8
225	npbverb	npbverb	Option to enable verbose output from the pbsa program	identifier	14
226	nrespa	nrespa	sander variable to enable multiple time-step integration (RESPA).	identifier	23
227	nsnba	nsnba	Frequency (in steps) for generating the atom-based non-bonded pairlist	identifier	4

228	ntave	ntave	sander variable for the frequency of printing running energy averages.	identifier	41
229	Periodic Boundary Conditions	ntb	Flag to control the use of periodic boundary conditions.	state|method	70
230	ntc	ntc	sander flag to select the SHAKE algorithm for bond constraints.	identifier	53
231	ntf	ntf	sander flag controlling which bonded force terms are evaluated.	identifier	47
232	ntpr	ntpr	sander variable for the frequency of printing energy information to mdout.	identifier	77
233	ntwr	ntwr	sander variable for the frequency of writing the restart file.	identifier	34
234	ntwx	ntwx	sander variable for the frequency of writing coordinates to the trajectory.	identifier	41
235	ntx	ntx	sander variable controlling how initial coordinates and velocities are read.	identifier	47
236	Onufriev-Bashford-Case radii	GB^OBC model I	Radii set for a specific Generalized Born model (OBC)	data source|model	0
237	OPC	OPC	A 4-site optimal point charge rigid water model	model|chemical entity	55
238	order	order	The order of the B-spline interpolation used in PME.	measure	348
239	outlvlset	outlvlset	Option to write the total level set function to a file	identifier	6
240	outmlvlset	outmlvlset	Option to write the membrane-only level set function to a file	identifier	4
241	packmol-memgen	packmol-memgen	A workflow to generate protein/membrane/solvent systems for Amber	software|process	24
242	ParmEd	ParmEd	A Python tool for editing Amber topology and parameter files.	software	123
243	Particle Mesh Ewald	PME	A fast algorithm for calculating long-range electrostatic interactions.	algorithm|method	121
244	Poisson-Boltzmann Calculation Type	PB	Specifies the type of Poisson-Boltzmann calculation to perform	method|identifier	168
245	PBSA	PBSA	A continuum solvation model based on the Poisson-Boltzmann equation	model|method	207
246	pbsa.cuda	pbsa.cuda	The GPU-accelerated version of the pbsa program	software	18
247	pbtemp	pbtemp	Temperature in Kelvin used for the PB equation	identifier|measure	2
248	pdb4amber	pdb4amber	A program to analyze and clean PDB files for use in Amber	software	21
249	force field	pGM	A polarizable force field using distributed multipoles.	model	39
250	Constant pH REMD	pH-REMD	REMD where replicas are simulated at different constant pH values.	method|algorithm	41
251	phiform	phiform	Option to control the file format of the electrostatic potential map	identifier	9
252	phiout	phiout	Option to output the electrostatic potential map for visualization	identifier	7
253	PM3	PM3	Parameterization Method 3, a semi-empirical quantum mechanics method	model|method	57
254	pmemd	pmemd	High-performance parallel molecular dynamics simulation program	software|algorithm	367
255	pmemd.cuda	pmemd.cuda	GPU-accelerated version of the pmemd program using CUDA	software|algorithm	71
256	Poisson-Boltzmann equation	equation	A differential equation describing electrostatic potential in an ionic solution	model|method	6
257	Polar Decomposition	polarDecomp	Decomposes solvation free energy into polar and non-polar parts	method|process	17
258	Polarizable Force Field	polarizable	A force field that accounts for induced electronic polarization	model	42
259	poretype	poretype	Option to enable an automatic pore-finding algorithm in membranes	identifier	6
260	powell	powell	An optimization method available in SciPy for parameter fitting.	algorithm|method	3
261	PQR file	PQR	A file format similar to PDB but with charge (Q) and radius (R) columns.	data format	35
262	prep file	.prep	An Amber file format containing residue information, used by GLYCAM	data format	6
263	Topology File	prmtop	An Amber file format containing force field parameters and topology	data format	519
264	progress	progress	Keyword in rism1d for the frequency of reporting the residual	identifier	21
265	PropPDB	PropPDB	A program to propagate a crystal unit cell to create a supercell.	software	6

266	ProScrs.py	ProScrs.py	A program called 'Protein Scissors' for cutting and capping protein segments.	software	13
267	py_resp.py	py_resp.py	A Python program for electrostatic potential (ESP) fitting.	software	35
268	PyMol	PyMol	A molecular visualization system	software	18
269	pyMSMT	pyMSMT	Tool to build and validate models of metalloproteins	software|method	7
270	pype-resp.py	pype-resp.py	A pipeline to facilitate and standardize the derivation of RESP charges.	software|process	26
271	pyresp_gen.py	pyresp_gen.py	A program to automatically generate input files for py_resp.py.	software	18
272	pytraj	pytraj	A Python library that provides a front-end to the cpptraj analysis engine	software	32
273	QM Atom Indices	iqmatoms	A list of atom numbers defining the atoms in the QM region	identifier	9
274	QM SHAKE	qmshake	Controls whether the SHAKE algorithm is applied to QM atoms	state|method	7
275	QM/MM Switching Function	qmmm_switch	A function to smoothly transition the potential at the cutoff	method	8
276	QM/MM+ΔMLP	QM/MM+ΔMLP	A QM/MM model corrected by a machine learning potential	model|method	0
277	Semi-empirical Hamiltonian	qm_theory	An approximation to the exact quantum mechanical Hamiltonian	model	46
278	QM Charge	qmcharge	The total integer charge of the quantum mechanical region	measure	25
279	QM/MM Cutoff	qmcut	The cutoff distance for non-bonded interactions involving the QM region	measure|unit	24
280	QM Generalized Born Treatment	qmgb	Specifies how the QM region is treated with Generalized Born.	method|model	6
281	Dynamical QM Region	qmmask	Atoms that follow QM forces during dynamics	model	52
282	QM/MM Interaction Scheme	qmmm_int	Controls how direct-space QM/MM electrostatic interactions are calculated	model	19
283	r-RESPA	rismnrespa	Reversible reference system propagator algorithm for multiple time-stepping	algorithm|method	24
284	R6 integration	R6 integration	A numerical integration method over the molecular surface for Born radii	method|algorithm	0
285	radiopt	radiopt	Option to select the source of atomic radii for PB calculations	identifier	21
286	RATTLE	RATTLE	An algorithm for constraining bond velocities in dynamics simulations.	algorithm|method	5
287	rbornstat	rbornstat	Flag to report statistics of effective Born radii during simulation	identifier	5
288	RDKit	RDKit	An open-source cheminformatics software toolkit used by pype-resp.py.	software|library	3
289	rdt	rdt	A parameter for GB simulations with Locally Enhanced Sampling (LES)	identifier|measure	10
290	REMD Log File	rem.log	Default log file name containing information about replica exchanges.	data format|data source	20
291	Replica Exchange Molecular Dynamics	REMD	states.	method|algorithm	325
292	Dynamics	RXSGLD	Combines REMD with Self-Guided Langevin Dynamics for enhanced sampling.	method|algorithm	22
293	RESP	RESP	Restrained Electrostatic Potential fit, a method for deriving atomic charges	method|model	161
294	RESP-ind	RESP-ind	A RESP model that includes atomic induced dipoles.	model|method	13
295	RESP-perm	RESP-perm	A RESP model that includes permanent atomic dipoles.	model|method	20
296	Restart File	--rst	File containing coordinates and velocities for restarting a simulation	data format	55
297	Restart File	restrt	An Amber file format containing coordinates, velocities, and box vectors	data format	92
298	rgbmax	rgbmax	Maximum distance for pairwise summation in Born radii calculation	identifier|measure	13
299	rhow_effect	rhow_effect	Effective water density for the non-polar dispersion term calculation	identifier|measure	1
300	3D-RISM Solvation Energy	rism	The total solvation free energy from 3D-RISM calculations.	measure	266
301	rism3d.snglpnt	rism3d.snglpnt	A standalone program for single-point 3D-RISM calculations	software	24
302	Salt Concentration	saltcon	Molar salt concentration for implicit solvent models.	measure|state	57
303	sander	sander	Basic energy minimization and molecular dynamics program in AmberTools	software|algorithm	624

304	Sander API	sander_api	Application Programming Interface for the sander program.	software	8
305	saopt	saopt	Option to enable the calculation of the molecular surface area	identifier	4
306	Solvent Accessible Surface Area	SASA	The surface area of a biomolecule accessible to solvent	measure	61
307	sasopt	sasopt	Option to select the type of molecular surface to be used	identifier	17
308	saveAmberParm	saveAmberParm	LEaP command to save topology and coordinate files for Amber	software	22
309	savepdb	savepdb	LEaP command to save a Protein Data Bank (PDB) file.	software|process	9
310	scale	scale	ParmEd command to scale all values in a specific prmtop section.	software|process	117
311	scalec	scalec	Option to scale dielectric boundary surface charges	identifier	2
312	SCF Convergence Criteria	scfconv	The energy threshold for self-consistent field (SCF) convergence	measure	23
313	GaMD Soft Core Mask	scmask1	Amber mask specifying atoms to be treated with soft core potentials.	identifier|data format	23
314	Seminario method	sem	A method to derive force constants from a Cartesian Hessian matrix.	method|algorithm	19
315	sequence	sequence	LEaP command to combine and bond a list of units into a new unit	software	107
316	SIRAH force field	SIRAH	A residue-based coarse-grained force field for biomolecules	model	29
317	slsqp	slsqp	Sequential Least Squares Programming, an optimization method used by OptC4.py.	algorithm|method	1
318	SLTCAP method	SLTCAP method	Method to calculate the number of ions to add for a target concentration	method	1
319	SMARTS	SMARTS	A language for specifying molecular substructures for atom selection.	identifier|model	17
320	smoothopt	smoothopt	Option for setting dielectric values at the solute-solvent boundary	identifier	9
321	Solute Dielectric Constant	epsin	The dielectric constant inside the solute molecule for PBSA calculations	measure|model	31
322	solvateBox	solvateBox	LEaP command to create a periodic rectangular solvent box around a solute	software	16
323	solvateOct	solvateOct	LEaP command to create a periodic truncated octahedron solvent box	software	13
324	solvbox	solvbox	Keyword to set the dimensions of a fixed-size solvent box	identifier|measure	32
325	solvopt	solvopt	Option to select the iterative solver for the PB equation	identifier	15
326	space	space	The grid spacing for the finite-difference solver	identifier|measure	1776
327	space group	space group	The set of symmetry operations that describes a crystal structure.	model|identifier	5
328	SPC/E	SPC/E	A 3-site extended simple point charge rigid water model	model|chemical entity	30
329	Spin Multiplicity	spin	Specifies the spin state of the QM system (e.g., singlet, doublet)	state	28
330	sprob	sprob	Solvent probe radius for SASA used in the dispersion term	identifier|measure	4
331	sqm	sqm	A semi-empirical quantum mechanics program included in AmberTools.	software	31
332	Steered Molecular Dynamics	SMD	A method where an external force is applied to drive a system along a coordinate.	method|process	30
333	surften	surften	Surface tension parameter for the nonpolar solvation energy calculation	identifier|measure	8
334	sviol	sviol	A script that summarizes energies and restraint violations from sander output	software	3
335	Swarms-of-Trajectories String Method	STSM	A path-finding algorithm to find the Minimum Free Energy Path	method|algorithm	21
336	Target Temperature	temp0	The target temperature for a replica in a T-REMD simulation.	measure|state	92
337	Temperature REMD	T-REMD	REMD where replicas are simulated at different temperatures.	method|algorithm	56
338	TER record	TER	A record in a PDB file separating non-covalently connected chains	data format	29
339	TeraChem	TeraChem	A GPU-accelerated quantum chemistry software for large molecular systems	software	58
340	Thermodynamic Integration	TI	A free energy method calculating dG by integrating over lambda	method|model	182
341	GaMD Ligand/Peptide Mask	timask1	Amber mask specifying atoms of the ligand, peptide, or protein.	identifier|data format	19

342	Time-averaged restraints	Time-averaged restraints	Restraints applied to the time-averaged value of an internal coordinate	method|model	7
343	tiMerge	tiMerge	ParmEd command to merge two topologies for a thermodynamic integration calculation.	software|process	4
344	TIP3P	TIP3P	A common 3-site water model used in simulations.	model	68
345	tolerance	tolerance	The convergence criterion for the self-consistent solution in 3D-RISM	measure	105
346	Torch PBSA runtime	Torch PBSA runtime	A dedicated C++ runtime using LibTorch for PBSA calculations	software	8
347	triopt	triopt	Option to use trimer arc dots for more accurate surface mapping	identifier	5
348	UnitCell	UnitCell	A program to reconstruct a complete crystal unit cell from a PDB file.	software	8
349	Urey-Bradley Term	Urey-Bradley	A 1-3 non-bonded interaction term used in CHARMM force fields.	model	21
350	use_rmin	use_rmin	Option to use rmin values for van der Waals radii	identifier	3
351	use_sav	use_sav	Option to use molecular volume or surface area for the cavity term	identifier	7
352	Van der Waals Energy	vdw	The van der Waals contribution to the total energy.	measure	122
353	Verbose Level	verbose	Controls the amount of diagnostic output to the log file	state	48
354	VMD	VMD	A molecular visualization program	software	31
355	vprob	vprob	Solvent probe radius for molecular volume used in the cavity term	identifier|measure	2
356	Level Shifting	vshift	Shifts virtual orbital energies to improve SCF convergence	method	8
357	Well-Tempered ABMD	WT-ABMD	An ABMD variant with a non-uniform update rate for smoother convergence.	method|algorithm	7
358	xleap	xleap	The X-windows graphical user interface version of LEaP	software	12
359	xmax	xmax	The upper boundary of the active site focusing box in x	identifier|measure	3
360	xvv file	.xvv	An output file from 1D-RISM containing bulk solvent properties	data format	16
361	Z-matrix method	zmx	A method to generate force field parameters using a Z-matrix.	method|algorithm	7
362	α_k	α_k	Fractional solvent accessible surface area in the GTFE model	measure	0
363	Surface Tension	γ	Parameter representing the surface tension in nonpolar energy calculations	measure|model	29
364	ΔG_tr	ΔG_tr	The free energy of transfer term in the GTFE model	measure	0
365	Δg_tr,k	Δg_tr,k	Group transfer free energies for sidechains or backbone in GTFE	measure	0
366	Lambda	λ	The coupling parameter that controls the alchemical transformation state	measure|state	326
367	Amber	Amber	Suite of programs for carrying out molecular dynamics simulations	software|model	970
368	AmberTools25	AmberTools25	A collection of freely available programs for Amber	software	10
369	Amber24	Amber24	Licensed simulation program component centered around pmemd	software	16
370	Force Field	force field	Empirical potential energy function for molecular systems	model	301
371	PDB Format	PDB format	Standard file format for 3D biomolecular structures	data format	20
372	Residue Library	Residue libraries	Database of molecular topology, atom names, and charges	data source|model	5
373	prmcrd	prmcrd	Amber coordinate file for a molecular system	data format	4
374	AMOEBA	AMOEBA	A polarizable force field for biomolecular simulations	model	37
375	GEM	GEM	A polarizable force field based on the Gaussian Electrostatic Model	model	47
376	CMake	CMake	Cross-platform build system used to compile the Amber software	software	86
377	AMBERHOME	$AMBERHOME	Environment variable pointing to the Amber installation directory	identifier	298
378	MPI (Message Passing Interface)	MPI	A standard for parallel computing using message passing	software|method	194
379	OpenMP	OpenMP	An API for shared-memory parallel programming	software|method	25

380	ROCm	ROCm	AMD's software stack for GPU programming	software|method	7
381	BLAS	BLAS	A specification for low-level matrix and vector operations	software|method	14
382	LAPACK	LAPACK	A library providing routines for high-level linear algebra operations	software|method	16
383	MKL	MKL	Intel's Math Kernel Library of optimized math routines	software	23
384	Miniconda	Miniconda	A minimal installer for the conda package and environment manager	software	6
385	update_amber	update_amber	A Python script to manage updates for the Amber source code	software	26
386	ff19SB	ff19SB	Protein force field with improved amino-acid-specific backbone parameters	model	56
387	OL24	OL24	Recommended DNA force field with refined sugar pucker dihedrals	model	7
388	OL3	OL3	Recommended RNA force field with glycosidic torsion corrections	model	5
389	GLYCAM_06j	GLYCAM_06j	A transferable parameter set for modeling carbohydrates	model	17
390	tip4pew	tip4pew	A four-site water model optimized for use with Ewald sums	model|chemical entity	13
391	ff14SB	ff14SB	Protein force field with refined backbone and sidechain parameters	model	56
392	ff99SB	ff99SB	Protein force field with reparametrized backbone torsion terms	model	20
393	ff15ipq	ff15ipq	Protein force field using iteratively derived IPolQ charges	model	23
394	SPC/E-b	SPC/E-b	A three-point water model by Takemura and Kitao	model|chemical entity	2
395	ff15ipq-m	ff15ipq-m	An expanded version of ff15ipq for protein mimetics	model	1
396	fb15	fb15	A protein force field derived using a force-balance approach	model|method	5
397	tip3pfb	tip3pfb	A three-point water model designed for the fb15 force field	model|chemical entity	3
398	ff03	ff03	A protein force field with charges derived in a continuum solvent	model	16
399	ff03ua	ff03ua	A united-atom version of the ff03 protein force field	model	2
400	United-atom model	united-atom	A force field representation where nonpolar hydrogens are implicit	model|method	4
401	Intrinsically Disordered Proteins	proteins (IDPs)	Proteins lacking a stable tertiary structure	chemical entity|state	3
402	ff99-bsc0	ff99-bsc0	A nucleic acid force field with alpha/gamma torsion corrections	model	4
403	OL15	OL15	A DNA force field combining several dihedral angle corrections	model	6
404	bsc1	bsc1	An updated nucleic acid force field for alpha/gamma torsions	model	6
405	tumuc1	tumuc1	A DNA force field with refined QM-based electrostatic parameters	model	4
406	OL21	OL21	A DNA force field that builds upon OL15 with corrections	model	4
407	Phosphorylated Amino Acid	acids	Amino acids chemically modified with a phosphate group	chemical entity	5
408	phosaa10	leaprc.phosaa10	Parameters for phosphorylated amino acids for older force fields	model|data source	2
409	phosaa14SB	leaprc.phosaa14SB	Parameters for phosphorylated amino acids compatible with ff14SB	model|data source	2
410	phosaa19SB	leaprc.phosaa19SB	Parameters for phosphorylated amino acids compatible with ff19SB	model|data source	2
411	modXNA	modXNA	A tool to create new Amber-compatible modified nucleotide structures	software|method	15
412	GLYCAM06	GLYCAM06	A transferable parameter set for modeling carbohydrates and glycoconjugates	model	6
413	GLYCAM06EP	GLYCAM06EP	A GLYCAM version with extra points for TIP5P water model	model	1
414	Extra Points	Extra points (EPs)	Off-atom sites representing lone pair electrons in force fields	model|method	13
415	Partial Atomic Charge	partial charges	A charge value assigned to an individual atom in a molecule	measure|model	47
416	Implicit Solvent Model	implicit solvent model	A continuum representation of solvent effects in simulations	model|method	10
417	Ramachandran Map	Ramachandran map	A plot showing allowed regions for protein backbone dihedral angles	measure|data source	1

418	D-Arabinose	d-Arabinose	A five-carbon aldose sugar, a type of monosaccharide	chemical entity	0
419	D-Lyxose	d-Lyxose	A five-carbon aldose sugar, an epimer of D-xylose	chemical entity	0
420	D-Ribose	d-Ribose	A five-carbon aldose sugar, a component of RNA	chemical entity	0
421	D-Xylose	d-Xylose	A five-carbon aldose sugar, also known as wood sugar	chemical entity	0
422	D-Allose	d-Allose	A six-carbon aldose sugar, an epimer of glucose	chemical entity	0
423	D-Altrose	d-Altrose	A six-carbon aldose sugar, an epimer of mannose	chemical entity	0
424	D-Galactose	d-Galactose	A six-carbon aldose sugar, a component of lactose	chemical entity	0
425	D-Glucose	d-Glucose	A six-carbon aldose sugar, a primary source of energy	chemical entity	0
426	D-Gulose	d-Gulose	A six-carbon aldose sugar, an epimer of galactose	chemical entity	0
427	D-Idose	d-Idose	A six-carbon aldose sugar, an epimer of gulose	chemical entity	0
428	D-Mannose	d-Mannose	A six-carbon aldose sugar, an epimer of glucose	chemical entity	0
429	D-Talose	d-Talose	A six-carbon aldose sugar, an epimer of galactose	chemical entity	0
430	D-Fructose	d-Fructose	A six-carbon ketose sugar, commonly found in fruits	chemical entity	0
431	D-Psicose	d-Psicose	A six-carbon ketose sugar, a low-calorie sweetener	chemical entity	0
432	D-Sorbose	d-Sorbose	A six-carbon ketose sugar, used in vitamin C synthesis	chemical entity	0
433	D-Tagatose	d-Tagatose	A six-carbon ketose sugar, a low-calorie sweetener	chemical entity	0
434	D-Fucose	d-Fucose	A six-carbon deoxy sugar, a component of glycoproteins	chemical entity	0
435	D-Quinovose	d-Quinovose	A six-carbon deoxy sugar, found in plant glycosides	chemical entity	0
436	D-Rhamnose	d-Rhamnose	A six-carbon deoxy sugar, found in plant glycosides	chemical entity	0
437	D-Galacturonic Acid	d-Galacturonic Acid	An oxidized form of galactose, a component of pectin	chemical entity	0
438	D-Glucuronic Acid	d-Glucuronic Acid	An oxidized form of glucose, involved in detoxification	chemical entity	0
439	D-Iduronic Acid	d-Iduronic Acid	An oxidized form of idose, a component of glycosaminoglycans	chemical entity	0
440	D-N-Acetylgalactosamine	d-N-Acetylgalactosamine	An acetylated amino sugar derived from galactose	chemical entity	0
441	D-N-Acetylglucosamine	d-N-Acetylglucosamine	An acetylated amino sugar derived from glucose, component of chitin	chemical entity	0
442	D-N-Acetylmannosamine	d-N-Acetylmannosamine	An acetylated amino sugar derived from mannose	chemical entity	0
443	N-Acetyl-neuraminic Acid	N-Acetyl-neuraminic Acid	A type of sialic acid found in glycoproteins	chemical entity	0
444	KDN	KDN	Deaminated neuraminic acid, a type of sialic acid	chemical entity	3
445	KDO	KDO	3-deoxy-D-manno-oct-2-ulosonic acid, a component of lipopolysaccharides	chemical entity	3
446	N-Glycolyl-neuraminic Acid	Acid	A type of sialic acid found in many mammals	chemical entity	0
447	GLYCAM residue name	0GA, 0LB, 1GA, etc.	Three-letter code for carbohydrate residues in GLYCAM force field	identifier	0
448	prepareforleap	prepareforleap	An action in cpptraj to prepare carbohydrate PDB files	software|process	2
449	LIPID11	LIPID11	An early modular Amber lipid force field from 2011	model	5
450	GAFFLipid	GAFFLipid	A lipid parameter set based on the General Amber Force Field	model	2
451	LIPID14	LIPID14	An Amber lipid force field for tensionless NPT simulations	model	13
452	LIPID17	LIPID17	An extension of LIPID14 with more head and tail groups	model	5
453	Lauroyl (12:0)	LAL	A saturated 12-carbon fatty acyl chain residue	chemical entity|identifier	2
454	Myristoyl (14:0)	MY	A saturated 14-carbon fatty acyl chain residue	chemical entity|identifier	11
455	Palmitoyl (16:0)	PA	A saturated 16-carbon fatty acyl chain residue	chemical entity|identifier	9

456	Sphingosine (16:1)	SA	An 18-carbon amino alcohol with an unsaturated hydrocarbon chain	chemical entity|identifier	23
457	Oleoyl (18:1 n-9)	OL	A monounsaturated 18-carbon fatty acyl chain residue	chemical entity|identifier	5
458	Stearoyl (18:0)	ST	A saturated 18-carbon fatty acyl chain residue	chemical entity|identifier	2
459	Arachidonoyl (20:4)	AR	A polyunsaturated 20-carbon fatty acyl chain residue	chemical entity|identifier	15
460	Docosahexaenoyl (22:6)	DHA	A polyunsaturated 22-carbon fatty acyl chain residue	chemical entity|identifier	2
461	Phosphatidylcholine	PC	A class of phospholipids incorporating choline as a headgroup	chemical entity|identifier	18
462	Phosphatidylethanolamine	PE	A class of phospholipids with an ethanolamine headgroup	chemical entity|identifier	7
463	Phosphatidylserine	PS	A class of phospholipids with a serine headgroup	chemical entity|identifier	60
464	Phosphatidylglycerol (R-)	PGR	A class of phospholipids with an R-glycerol headgroup	chemical entity|identifier	2
465	Phosphatidylglycerol (S-)	PGS	A class of phospholipids with an S-glycerol headgroup	chemical entity|identifier	2
466	Phosphaditic acid	PH-	A simple phospholipid with a free phosphate headgroup	chemical entity|identifier	6
467	Sphingomyelin	SPM	A type of sphingolipid found in animal cell membranes	chemical entity|identifier	3
468	Cholesterol	CHL	A sterol lipid essential for animal cell membranes	chemical entity|identifier	6
469	CONECT records	CONECT records	Records in a PDB file specifying atomic connectivity	data format	2
470	TIP4P/Ew	TIP4P/Ew	A 4-site rigid water model optimized for Ewald sums	model|chemical entity	6
471	OPC3	OPC3	A 3-site optimal point charge rigid water model	model|chemical entity	38
472	OPC3-pol	OPC3-pol	A 3-site polarizable water model based on a Drude oscillator	model|chemical entity	21
473	solvents.lib	solvents.lib	An Amber library file containing various solvent models	data source	4
474	frcmod.tip4pew	frcmod.tip4pew	Force field modification file for the TIP4P/Ew water model	data format|data source	1
475	Drude oscillator	Drude oscillator	A model for electronic polarizability using a charged, massless particle	model|method	1
476	Joung/Cheatham ion parameters	frcmod.ionsjc_tip3p	A consistent set of parameters for alkali and halide ions	model|data source	6
477	Li/Merz ion parameters	p	Ion parameters developed to reproduce HFE, IOD, and CN values	model|data source	13
478	12-6-4 LJ-type nonbonded model	nonbonded model	A nonbonded potential including an r^{-4} term for polarization effects	model	4
479	Hydration Free Energy (HFE)	(HFE)	The free energy change of transferring an ion from vacuum to water	measure	1
480	Ion-Oxygen Distance (IOD)	(IOD)	The average distance between an ion and water oxygen atoms	measure	1
481	Coordination Number (CN)	(CN)	The average number of water molecules in an ion's first solvation shell	measure	2
482	ParmAM1	ParmAM1	A classical force field that reproduces AM1-minimized geometries	model	1
483	parmPM3	parmPM3	A classical force field that reproduces PM3-minimized geometries	model	1
484	GAL17 force field	GAL17	A force field for the interaction of water and a Pt(111) surface	model	9
485	&music namelist	&music	An input namelist in sander for the GAL17 force field	data format|identifier	2
486	belly dynamics	belly	A simulation where a subset of atoms is restrained	method	7
487	AMBER-DYES	AMBER-DYES	A force field for commonly used fluorescent dyes and linkers	model	9
488	leaprc.amberdyes	leaprc.amberdyes	The LEaP resource file for loading the AMBER-DYES force field	data format|data source	3
489	FRET	FRET	Forster Resonance Energy Transfer, an experimental distance measurement technique	method|measure	12
490	Alexa Fluor 350	A35	A blue-fluorescent dye	chemical entity|identifier	2
491	ATTO 488	T48	A green-fluorescent dye	chemical entity|identifier	2
492	Lumiprope Cy3	C3N	A cyanine-based fluorescent dye	chemical entity|identifier	2
493	Fluorescent chromophore	CRO, IIC, etc.	The light-absorbing and emitting part of a fluorescent protein	chemical entity|identifier	0

494	leaprc.xFPchromophores	leaprc.xFPchromophores	LEaP resource file for fluorescent protein chromophore parameters	data format|data source	1
495	Coarse-Grained (CG)	Coarse-Grained (CG)	A simplified molecular representation with fewer degrees of freedom	model|method	1
496	Multiscale simulation	Multiscale simulations	A simulation combining different levels of model resolution	method	5
497	WatFour (WT4)	WT4	The explicit coarse-grained water model for the SIRAH force field	model|chemical entity	3
498	Backmapping	Backmapping	The process of reconstructing an all-atom model from a CG model	process|method	3
499	cgconv.pl	cgconv.pl	A Perl script for converting all-atom PDBs to SIRAH CG PDBs	software|process	2
500	leaprc.sirah	leaprc.sirah	The LEaP resource file for loading the SIRAH force field	data format|data source	2
501	Generalized Born (GB) model	Generalized Born (GB)	An implicit solvent model approximating continuum electrostatic effects	model|method	7
502	Solvent Accessible Surface Area (SA)	Surface Area	A measure of the molecular surface exposed to solvent	measure|model	41
503	Effective Born radius	R_i	A parameter in GB models representing the degree of an atom's burial	measure|model	6
504	OBC model	igb=2, igb=5	Onufriev-Bashford-Case generalized Born models	model|identifier	1
505	GBn model	igb=7, igb=8	A newer generation of generalized Born models	model|identifier	2
506	PBradii	PBRadii	A LEaP command to set the set of atomic radii for GB/PB calculations	identifier|data source	18
507	extdiel	extdiel	Input parameter for the solvent's exterior dielectric constant	identifier|measure	9
508	1D-RISM	1D-RISM	A version of RISM for calculating bulk solvent properties	model|method	37
509	rism1d	rism1d	The executable program for 1D-RISM calculations	software	31
510	Ornstein-Zernike (OZ) equation	equation	An integral equation relating correlation functions in a fluid	model|method	0
511	total correlation function	h	A function describing the total correlation between two particles	measure	379
512	direct correlation function	c	A function describing the direct correlation between two particles	measure	870
513	pair-distribution function	g_ab	Gives the conditional probability of finding a particle at a distance from another	measure	2
514	PSE-n	PSE-n	A closure relation that interpolates between KH and HNC	model|method	5
515	intramolecular pair correlation matrix	ω_αγ(k)	A function describing the correlation between sites within the same molecule	measure|model	2
516	DRISM	DRISM	Dielectrically consistent RISM theory	model|method	8
517	mean solvation force	f_i^UV(R_i)	The average force exerted by the solvent on a solute atom	measure	2
518	Gaussian fluctuation (GF) approximation	GF	An alternative approximation for the solvation free energy	model|method	12
519	Treecode	Treecode	A fast summation method for calculating long-range interactions	algorithm|method	43
520	force-coordinate extrapolation (FCE)	FCE	A multiple time step method that extrapolates forces	algorithm|method	15
521	FCEstride	FCEstride	Input variable for the FCE outer time step	identifier|measure	8
522	FCEnbase	FCEnbase	Input variable for the number of previous solutions used for FCE	identifier|measure	11
523	centering	centering	Keyword to control how the solute is centered in the solvent box	identifier	87
524	gfCorrection	gfCorrection	Keyword to enable calculation of the GF excess chemical potential	identifier	2
525	pcpluscorrection	pcpluscorrection	Keyword to enable calculation of the PC+/3D-RISM excess chemical potential	identifier	1
526	uccoeff	uccoeff	Keyword to provide coefficients for the UC excess chemical potential	identifier|measure	3
527	periodic	periodic	Keyword to enable periodic boundary conditions in 3D-RISM	identifier	166
528	asympcorr	asympcorr	Keyword to enable long-range asymptotic corrections	identifier	2
529	treeDCF	treeDCF	Keyword to enable treecode approximation for the direct correlation function	identifier	4
530	treeTCF	treeTCF	Keyword to enable treecode approximation for the total correlation function	identifier	4
531	treeCoulomb	treeCoulomb	Keyword to enable treecode approximation for the Coulomb potential	identifier	4

532	treeDCFMAC	treeDCFMAC	Treecode MAC parameter for the direct correlation function	identifier|measure	4
533	treeTCFMAC	treeTCFMAC	Treecode MAC parameter for the total correlation function	identifier|measure	4
534	treeCoulombMAC	treeCoulombMAC	Treecode MAC parameter for the Coulomb potential	identifier|measure	4
535	treeDCFOrder	treeDCFOrder	Treecode Taylor series order for the direct correlation function	identifier|measure	4
536	treeTCFOrder	treeTCFOrder	Treecode Taylor series order for the total correlation function	identifier|measure	4
537	treeCoulombOrder	treeCoulombOrder	Treecode Taylor series order for the Coulomb potential	identifier|measure	4
538	treeDCFN0	treeDCFN0	Treecode maximum leaf size for the direct correlation function	identifier|measure	4
539	treeTCFN0	treeTCFN0	Treecode maximum leaf size for the total correlation function	identifier|measure	4
540	treeCoulombN0	treeCoulombN0	Treecode maximum leaf size for the Coulomb potential	identifier|measure	4
541	ng3	ng3	Keyword to set the number of grid points for a fixed-size box	identifier|measure	3
542	ljTolerance	ljTolerance	Keyword to determine the Lennard-Jones cutoff distance	identifier|measure	23
543	asympKSpaceTolerance	asympKSpaceTolerance	Keyword to determine the reciprocal space long-range asymptotics cutoff	identifier|measure	10
544	mdiis_nvec	mdiis_nvec	Keyword for the number of MDIIS vectors	identifier|measure	12
545	maxstep	maxstep	Keyword for the maximum number of iterations for the RISM solver	identifier|measure	10
546	npropagate	npropagate	Keyword for the number of previous solutions to use as an initial guess	identifier|measure	10
547	zerofrc	zerofrc	Keyword to control the redistribution of solvent forces	identifier	2
548	apply_rism_force	apply_rism_force	Keyword to enable/disable calculation of RISM solvation forces	identifier	2
549	fcesort	fcesort	Keyword to enable sorting of FCE basis vectors	identifier	2
550	fcecrd	fcecrd	Keyword to select the coordinate system for the FCE method	identifier	3
551	fceweigh	fceweigh	Keyword to enable weighted coordinates for force extrapolation	identifier	2
552	fceenormsw	fceenormsw	Keyword for the balancing parameter in ASFE extrapolation	identifier|measure	4
553	fcetrans	fcetrans	Keyword to select the FCE transformation and extrapolation method	identifier	10
554	fceifreq	fceifreq	Keyword for the mapping list updating frequency in GSFE schemes	identifier|measure	6
555	fcentfrcor	fcentfrcor	Keyword for the net force correction flag in GSFE schemes	identifier	3
556	ntwrism	ntwrism	Keyword for the frequency of writing solvent density grids	identifier	6
557	molReconstruction	molReconstruction	Keyword to enable output of molecularly reconstructed thermodynamic distributions	identifier	2
558	theory	theory	Keyword in rism1d to select the 1D-RISM theory (DRISM or XRISM)	identifier	91
559	dr	dr	Keyword in rism1d for the real space grid spacing	identifier|measure	16
560	nr	nr	Keyword in rism1d for the number of grid points	identifier|measure	12
561	outlist	outlist	Keyword in rism1d to specify which output files to produce	identifier	3
562	rout	rout	Keyword in rism1d for the maximum real space output distance	identifier|measure	2
563	kout	kout	Keyword in rism1d for the maximum reciprocal space output distance	identifier|measure	2
564	ksave	ksave	Keyword in rism1d for the frequency of writing intermediate restart files	identifier	5
565	selftest	selftest	Keyword in rism1d to perform a self-consistency check	identifier	2
566	density	density	Keyword in rism1d species namelist for the species density	identifier|measure	169
567	units	units	Keyword in rism1d species namelist for the density units	identifier	114
568	model	model	Keyword in rism1d species namelist for the path to the .mdl file	identifier	563
569	extra_precision	extra_precision	Keyword in rism1d to control the use of extra precision routines	identifier	2

570	temperature	temperature	Keyword in rism1d for the temperature in Kelvin	identifier|measure	270
571	dieps	dieps	Keyword in rism1d for the dielectric constant of the solvent	identifier|measure	3
572	nsp	nsp	Keyword in rism1d for the number of species in the solution	identifier|measure	7
573	smear	smear	Keyword in rism1d for the charge smear parameter	identifier|measure	5
574	adbcor	adbcor	Keyword in rism1d for a numeric parameter for DRISM	identifier|measure	3
575	Volumetric Data Format	--volfmt	Specifies the file format for 3D grid data	data format	2
576	ccp4	ccp4	A format for volumetric data, compatible with MRC	data format	18
577	dx	dx	Data Explorer format for volumetric data on regular grids	data format	66
578	xyzv	xyzv	A simple ASCII format for volumetric data (x-y-z-value)	data format	6
579	Write Thermodynamics	write_thermo	Option to print solvation thermodynamics output	process	2
580	Minimization	imin=1	Process to find the lowest energy conformation of a molecule	method|process	173
581	Trajectory Post-Processing	imin=5	Analysis of a saved trajectory of molecular coordinates	process	14
582	PDB file	--pdb	Protein Data Bank file containing atomic coordinates	data format	211
583	Trajectory File	--traj	File containing a series of atomic coordinate snapshots over time	data format	48
584	Solvent Pair Distribution File	--guv	Output file for 3D solvent pair distribution functions (g_uv)	data format	3
585	Solvent Direct Correlation File	--cuv	Output file for 3D solvent direct correlation functions (c_uv)	data format	1
586	Solvent Total Correlation File	--huv	Output file for 3D solvent total correlation functions (h_uv)	data format	1
587	Solvent Potential File	--uuv	Output file for 3D solvent potential energy files	data format	1
588	Long Range Asymptotics	--asymp	Real-space long-range corrections for correlation functions	method|model	10
589	Solvent Charge Density Distribution	--quv	Output file for 3D solvent charge density distributions	data format	2
590	Solvent Charge Distribution	--chgdist	Output file for 3D point charge distributions from solvent	data format	2
591	Solvation Energy	--solvene	The energy change associated with dissolving a solute in a solvent	measure	22
592	Solvation Entropy	--entropy	The entropy change associated with dissolving a solute in a solvent	measure	7
593	Gaussian Fluctuation	--exchemGF	A method to calculate excess chemical potential	method|model	13
594	PC+ Correction	--exchemPC+	A correction method for solvation free energy calculations	method|model	4
595	UC Correction	--exchemUC	A universal correction method for solvation free energy	method|model	5
596	Solute-Solvent Potential Energy	--potUV	Distribution files for solute-solvent potential energy	data format	4
597	Partial Series Expansion (PSE)	PSEn	A type of closure relation for the RISM equation	model|method	6
598	Ewald Summation	ewald	A method for calculating long-range electrostatic interactions	algorithm|method	101
599	Asymptotic Correction	--noasympcorr	Turns off long-range asymptotic corrections for thermodynamic output	state	19
600	Grid Spacing	--grdspc	The spacing between points in a 3D grid	measure|unit	48
601	Grid Points	--ng	The number of points in each dimension of a 3D grid	measure	52
602	MDL File Format	MDL	Solvent MoDeL file format using prmtop specification	data format	18
603	Site-site functionals format	.vv	File format for separation-dependent site-site pair functionals	data format	0
604	Total excess coordination number	.n00	File providing total excess coordination number around each solvent site	data format	3
605	Total excess charge	.q00	File providing total excess charge about each solvent site	data format	6
606	RM1	RM1	Recife Model 1, a semi-empirical Hamiltonian	model	6
607	MNDO	MNDO	Modified Neglect of Diatomic Overlap, a semi-empirical Hamiltonian	model	21

608	PDDG/PM3	PDDG/PM3	Pairwise Distance Directed Gaussian modification of PM3	model	2
609	MNDO/d	MNDO/d	MNDO Hamiltonian extended with d-orbitals	model	4
610	PM6	PM6	Parameterization Method 6, a semi-empirical Hamiltonian	model	12
611	DFTB	DFTB	Density-Functional based Tight-Binding method	method|model	111
612	SCC-DFTB	SCC-DFTB	Self-Consistent-Charge Density-Functional based Tight-Binding (DFTB2)	method|model	23
613	DFTB3	DFTB3	Third-order Self-Consistent-Charge Density-Functional based Tight-Binding	method|model	27
614	DFTB parameter files	.skf	Slater-Koster files containing parameters for DFTB calculations	data format|data source	2
615	Empirical Hydrogen Bond Correction	AM1-DH+	An empirical term added to correct for hydrogen bonding	model|method	1
616	&qmmm namelist	&qmmm	Namelist in Amber input files for controlling QM/MM calculations	data format	49
617	DFTB Slater-Koster Path	dftb_slko_path	Specifies the directory path to DFTB parameter files	identifier	3
618	DFTB Charge Type	dftb_chg	Selects the type of atomic charges to report from a DFTB calculation	state	5
619	Gradient Tolerance	grms_tol	The root-mean-square gradient threshold to terminate minimization	measure	6
620	External Point Charges	#EXCHARGES	An electric field generated by a set of point charges	model	4
621	QUICK	QUICK	A GPU-enabled ab initio and DFT quantum chemistry program	software	127
622	Hartree-Fock	HF	An ab initio electronic structure method	method|model	29
623	Density Functional Theory	DFT	A quantum mechanical method to investigate electronic structure	method|model	56
624	Local Density Approximation	LDA	A class of exchange-correlation functionals in DFT	model	2
625	Generalized Gradient Approximation	GGA	A class of exchange-correlation functionals in DFT	model	7
626	Hybrid-GGA Functional	Hybrid-GGA	A class of DFT functionals mixing Hartree-Fock exchange	model	1
627	Grimme Dispersion Correction	corrections	A family of empirical corrections for dispersion in DFT	model|method	1
628	Restricted Closed-Shell	Restricted closed-shell	A wavefunction type for systems where all electrons are paired	state	1
629	Unrestricted Open-Shell	Unrestricted open-shell	A wavefunction type for systems with unpaired electrons	state	1
630	Mulliken Charge Analysis	Mulliken charge analysis	A method for calculating partial atomic charges from a QM calculation	method	1
631	Molden Format	Molden format	A file format for visualizing molecular geometry and orbital data	data format	1
632	Gaussian Basis Set	BASIS=	A set of functions used to represent molecular orbitals in QM calculations	model	0
633	SG1 Grid	SG1 grid	A standard grid system used for numerical integration in DFT calculations	model	1
634	QM/MM Calculation	ifqnt=1	A hybrid simulation method combining Quantum and Molecular Mechanics	method|model	21
635	Electrostatic Embedding	qmmm_int=1	A QM/MM coupling scheme where MM charges polarize the QM region	method|model	13
636	Link Atom		An artificial atom (typically H) to saturate valency at a QM/MM boundary	model	24
637	PM3/MM	qmmm_int=3	A reformulated QM/MM interface potential for the PM3 Hamiltonian	model|method	4
638	Ewald for QM/MM	qm_ewald=1	An Ewald summation method adapted for QM/MM periodic simulations	method|model	1
639	PME for QM/MM	qm_pme=1	A Particle Mesh Ewald method for QM/MM periodic simulations	algorithm|method	0
640	Print Dipole Moment	printdipole	Controls the printing of the system's dipole moment	state|process	4
641	Write PDB	writepdb	Writes a PDB file of the selected QM region for verification	state|process	3
642	Solvent in QM region	vsolv	Controls the inclusion of solvent molecules into the QM region	state|method	22
643	Charge-dependent vdW corrections	qxd=.true.	A charge-dependent model for QM/MM van der Waals interactions	model|method	1
644	qxd parameters	qxd_s	Parameters for the charge-dependent exchange-dispersion vdW model	measure|model	3
645	External QM/MM Interface	qm_theory = 'EXTERN'	Interface to use external QM software packages with sander	software|method	5

646	ADF	ADF	Amsterdam Density Functional, a quantum chemistry software package	software	25
647	GAMESS-US	GAMESS-US	A general-purpose ab initio quantum chemistry software package	software	18
648	NWChem	NWChem	An open-source high-performance computational chemistry software package	software	6
649	Gaussian	Gaussian	A widely used commercial computational chemistry software package	software	194
650	Orca	Orca	A flexible and efficient quantum chemistry program package	software	33
651	Q-Chem	Q-Chem	A comprehensive ab initio quantum chemistry software package	software	19
652	MRCC	MRCC	A quantum chemistry program for high-accuracy coupled-cluster methods	software	33
653	Fireball	Fireball	A local-orbital DFT QM/MM software	software	29
654	PUPIL	PUPIL	A simulation framework for coupling multiple simulation codes	software	2
655	File-based interface (FBI)	File-based interface (FBI)	A method for coupling programs via file exchange and system calls	method|software	4
656	Client/server model	client/server model	A data communication model for coupling programs, used by TeraChem	method|software	3
657	TCPB-cpp	TCPB-cpp	TeraChem Protocol Buffers C++ client for the client/server model	software	11
658	&adf namelist	&adf	Namelist in the Amber input file for controlling the ADF program	data format	3
659	ZLM fit	zlmfit	A density fitting method used in the ADF program	method|algorithm	8
660	Becke integration grid	beckegrid	A numerical integration grid for DFT calculations, used by ADF	model|algorithm	4
661	&gms namelist	&gms	Namelist in the Amber input file for controlling the GAMESS-US program	data format	3
662	Lebedev grids	nleb	Angular grids used for numerical quadrature in DFT calculations	model|algorithm	4
663	CHELPG charges	chelpg	A method to derive atomic charges from the electrostatic potential	method|measure	5
664	&gau namelist	&gau	Namelist in the Amber input file for controlling the Gaussian program	data format	4
665	&orc namelist	&orc	Namelist in the Amber input file for controlling the Orca program	data format	3
666	&qc namelist	&qc	Namelist in the Amber input file for controlling the Q-Chem program	data format	3
667	Auxiliary basis set	auxbasis	A secondary basis set used in density fitting or RI methods	model|data source	5
668	&mrcc namelist	&mrcc	Namelist in the Amber input file for controlling the MRCC program	data format	7
669	Multilayer calculation	embed	A QM/QM/MM or higher-level embedding scheme available in MRCC	method|model	6
670	&fb namelist	&fb	Namelist in the Amber input file for controlling the Fireball program	data format	6
671	Fdata directory	Fdata	Directory containing basis set and interaction parameters for Fireball	data source|data format	9
672	DFTD3 dispersion correction	idftd3	Grimme's D3 empirical dispersion correction for DFT methods	model|method	7
673	QUICK QM/MM Interface (API)	qm_theory = 'quick'	An API-based interface to use the QUICK QM program with sander	software|method	1
674	Application programming interface (API)	API	A method for directly linking software libraries for communication	software|method	125
675	&quick namelist	&quick	Namelist in the Amber input file for controlling the QUICK program	data format	4
676	TeraChem QM/MM Interface (TCPB)	qm_theory = 'terachem'	A client-server interface to use the TeraChem QM program with sander	software|method	2
677	&tc namelist	&tc	Namelist in the Amber input file for controlling the TeraChem program	data format	7
678	xTB	xTB	A software package implementing semiempirical GFN-xTB methods	software	39
679	GFN1-xTB	GFN1-xTB	A semiempirical tight-binding quantum mechanics method	model|method	2
680	GFN2-xTB	GFN2-xTB	An accurate and broadly parametrized semiempirical tight-binding QM method	model|method	4
681	&xtb namelist	&xtb	Namelist in the Amber input file for controlling the xTB program	data format	3
682	Chemical hardness	mmhardness	A parameter tuning QM/MM electrostatics in the xTB interface	measure|model	8
683	DFTB+	DFTB+	A software package for performing DFTB calculations	software	34

684	&dftbplus namelist	&dftbplus	Namelist in the Amber input file for controlling the DFTB+ program	data format	3
685	Hydrogen-bond correction	hcorrection	An empirical correction for hydrogen bonds in DFTB+	model|method	4
686	SCF Mixer	mixer	Selects the SCF iteration mixing algorithm (e.g., BROYDEN, DIIS)	algorithm	3
687	D3 dispersion model	d3s8	Grimme's D3 dispersion model with various parameters	model|method	3
688	(DAS)	DAS	An accurate method for adaptive QM/MM simulations	method|model	2
689	Active Region (A)	RA	The central region treated with high-level QM in adaptive QM/MM	model	6
690	Transition Region (T)	RT	The intermediate region where molecules have partial QM/MM character	model	7
691	Environment Region (E)		The region treated purely with MM in adaptive QM/MM	model	1
692	Force Interpolation		A scheme to calculate forces as a weighted sum, avoiding energy derivatives	method|algorithm	5
693	Conserved Quantity	$\tilde{E}$	A modified energy that is conserved during force interpolation dynamics	measure	3
694	&vsolv namelist	&vsolv	Namelist for controlling solvent inclusion in the QM region	data format	8
695	&adqmmm namelist	&adqmmm	Namelist for controlling adaptive QM/MM simulation details	data format	7
696	Number of Partitions	n_partition	Defines the number of QM/MM partitions in adaptive QM/MM	measure	6
697	Book-keeping Term	calc_wbk	A correction term for energy conservation in force interpolation schemes	measure|model	3
698	Adaptive Buffered Force-Mixing QM/MM	abfQM/MM	A method using two force calculations to handle adaptive QM/MM boundaries	method|model	21
699	Extended System		The larger QM/MM calculation for forces on dynamical QM atoms	model	1
700	Reduced System		The smaller calculation (MM or smaller QM) for MM forces	model	3
701	Hysteretic Algorithm		An algorithm using inner and outer radii to prevent rapid region fluctuations	algorithm|method	1
702	Adaptive Thermostat	ntt=6	A thermostat that handles intrinsic heating/cooling in non-conservative dynamics	method|algorithm	1
703	abfQM/MM Activation	abfqmmm	Flag to activate the adaptive buffered force-mixing method	state	10
704	Core Region Radii	r_core_in, r_core_out	Inner and outer radii for determining the core extension region	measure|unit	0
705	QM Region Radii	r_qm_in, r_qm_out	Inner and outer radii for determining the qm extension region	measure|unit	0
706	Buffer Region Radii	r_buffer_in, r_buffer_out	Inner and outer radii for determining the buffer extension region	measure|unit	0
707	Cuttable Bond List File	cut_bond_list_file	File specifying which chemical bonds are allowed to be cut	data format|data source	2
708	SEBOMD	qm_theory = 'SEBOMD'	SemiEmpirical Born-Oppenheimer Molecular Dynamics simulation method	method|model	33
709	Divide and Conquer	method=1	A linear scaling strategy for large quantum mechanical systems	algorithm|method	5
710	Mulliken Ewald Summation	longrange=2	Ewald summation using Mulliken charges for long-range electrostatics	method|algorithm	1
711	PIF Correction	modif=PIF2	A correction to the PM3 Hamiltonian for intermolecular interactions	model|method	0
712	MAIS Correction	modif=MAIS1	A correction to the PM3 Hamiltonian for water and other elements	model|method	0
713	&sebomd namelist	&sebomd	Namelist containing parameters for a SEBOMD simulation	data format	3
714	Long Range Interaction Type	longrange	Selects the type of long-range interaction for periodic systems	state	3
715	Peptide Bond Correction	peptcorr	Flag to apply a force field correction to peptide bonds	state|method	2
716	ReaxFF/AMBER		A hybrid reactive/non-reactive force field molecular dynamics framework	method|model	12
717	ReaxFF	ReaxFF	A reactive force field that can model bond formation and breaking	model|method	90
718	PuReMD	PuReMD	An open-source reactive molecular dynamics package implementing ReaxFF	software	19
719	Bond Order	BO	A measure of the number of chemical bonds between two atoms in ReaxFF	measure|model	9
720	Charge Equilibration (QEq)	charge_method=0	A method to dynamically determine partial atomic charges in ReaxFF	method|model	1
721	Electronegativity Equalization (EE)	charge_method=1	A method to dynamically determine partial atomic charges in ReaxFF	method|model	1

722	ReaxFF Force Field File	ffield	File containing parameters for a ReaxFF simulation	data format|data source	8
723	&reaxff namelist	&reaxff	Namelist for controlling ReaxFF/AMBER simulations	data format	7
724	External Library Interface	iextpot=1	A feature to use external libraries for energy and force calculations	software|method	1
725	MBX	extprog='mbx'	A software package for MB-pol and MB-nrg many-body potentials	software|model	9
726	reduce	reduce	A program for adding and optimizing hydrogens in a PDB file	software	54
727	HIE	HIE	Residue name for epsilon-protonated Histidine	chemical entity|identifier	11
728	HID	HID	Residue name for delta-protonated Histidine	chemical entity|identifier	10
729	ASH	ASH	Residue name for the neutral form of Aspartic Acid	chemical entity|identifier	2
730	GLH	GLH	Residue name for the neutral form of Glutamic Acid	chemical entity|identifier	2
731	LYN	LYN	Residue name for the neutral form of Lysine	chemical entity|identifier	1
732	NHE	NHE	Residue name for a C-terminal amide capping group	chemical entity|identifier	6
733	pdb2pqr	pdb2pqr	A tool to prepare PDB files by adding hydrogens and assigning charges at a given pH	software	18
734	propka3	propka3	A program to predict pKa values of ionizable groups in proteins	software	2
735	gwh	gwh	A program to optimize the positions of hydrogens in water molecules	software	7
736	Memembed	Memembed	A program for orienting proteins in membranes	software	2
737	pdbremix	pdbremix	A tool to estimate system volume for packing	software	1
738	Packmol	Packmol	A program for packing molecules in defined regions of space	software	37
739	Lipid_ext	Lipid_ext	An extension of the Lipid17/21 force fields with new lipid types	model|data source	6
740	Cardiolipin	CLI	A type of phospholipid containing two phosphatidylglycerol backbones	chemical entity	4
741	Lysophospholipid	PE1	A lipid derivative where one fatty acid chain is removed	chemical entity	4
742	Ergosterol	ERG	A sterol found in fungi and protozoa	chemical entity	3
743	Stigmasterol	STI	A plant-derived sterol	chemical entity	2
744	Sitosterol	SIT	A plant-derived sterol	chemical entity	3
745	Campesterol	CAM	A plant-derived sterol	chemical entity	3
746	Phosphatidylinositol	PI	A class of lipids that are part of the cell membrane	chemical entity	70
747	memgen.parm	--memgen_parm	A parameter file for packmol-memgen with lipid properties	data format|data source	3
748	Area per lipid (APL)	APL	The average area a lipid molecule occupies in a bilayer	measure|unit	5
749	Gaussian-shaped constraints	--xygauss	Constraints to generate curved or buckled membranes	method|model	3
750	AMBAT	AMBAT	Amber Membrane Builder and Analysis Tool for bilayer systems	software	3
751	PREP input file		An older Amber file format for residue topology information	data format	3
752	PARM format parameter set		An older Amber file format for force field parameters	data format	0
753	Object File Format (OFF)		A file format used by LEaP to save and load objects like UNITs and PARMSETs	data format	1
754	loadPdb	loadPdb	LEaP command to load a structure from a Protein Data Bank file	software	26
755	Commands		Instructions given to LEaP to manipulate objects	software	123
756	Variables		Handles for accessing objects within LEaP	software	225
757	Objects		Fundamental entities in LEaP, such as ATOMs, RESIDUEs, and UNITs	software	40
758	ATOM	ATOM	A complex object in LEaP representing a chemical atom	software|chemical entity	1212
759	RESIDUE	RESIDUE	A complex object in LEaP representing a collection of atoms, like an amino acid	software|chemical entity	678

760	UNIT	UNIT	The most complex object in LEaP, containing RESIDUEs and ATOMs	software	286
761	PARMSET	PARMSET	An object in LEaP containing force field parameters	software|data source	10
762	Atom Name	name	A case-sensitive string property identifying an ATOM	identifier	1061
763	Atom Charge	charge	A number representing the electrostatic point charge of an ATOM	measure	495
764	Atom Position	position	A list of three numbers representing the Cartesian coordinates of an ATOM	measure	169
765	Residue Connection Atom	connect0	An atom in a residue used to form linkages to other residues	identifier	8
766	Unit Head Atom	head	The atom in a UNIT used for connection when joining units	identifier	42
767	Unit Tail Atom	tail	The atom in a UNIT used for connection when joining units	identifier	46
768	Bounding Box	box	A property of a UNIT defining the periodic box dimensions	measure|model	365
769	Solvent Cap	cap	A property of a UNIT defining a spherical region of solvent	model	61
770	Universe Editor	Universe Editor	The main window in xleap for command-line interaction	software	7
771	Unit Editor	Unit Editor	A graphical molecule editor within xleap	software	10
772	Atom Properties Editor	Atom Properties Editor	A tool in xleap for editing atom properties in a table format	software	7
773	Parmset Editor	Parmset Editor	A tool in xleap for editing force field parameter sets	software	5
774	addAtomTypes	addAtomTypes	LEaP command to define element and hybridization for atom types	software	4
775	addC4Pairwise	addC4Pairwise	Adds a pairwise 12-6-4 non-bonded interaction between two specific atoms	software|method	4
776	addC4Type	addC4Type	Adds a 12-6-4 non-bonded interaction based on atom types	software|method	4
777	addIons2	addIons2	A variant of addIons where solvent and solute are treated the same	software|method	5
778	addIonsRand	addIonsRand	LEaP command to add counterions by replacing random solvent molecules	software|method	7
779	addPath	addPath	LEaP command to add a directory to the file search path	software	6
780	addPdbAtomMap	addPdbAtomMap	LEaP command to map atom names from a PDB file to internal residue definitions	software	4
781	addPdbResMap	addPdbResMap	LEaP command to map residue names from a PDB file to LEaP variables	software	7
782	alias	alias	LEaP command to create a shortcut for a command or string	software	28
783	bondByDistance	bondByDistance	LEaP command to create bonds between all atoms within a certain distance	software	4
784	check	check	LEaP command to check a unit for inconsistencies	software	80
785	combine	combine	LEaP command to combine multiple units into a single unit without bonding them	software	21
786	copy	copy	LEaP command to create an exact duplicate of an object	software	79
787	createAtom	createAtom	LEaP command to create a new ATOM object	software	8
788	createResidue	createResidue	LEaP command to create a new RESIDUE object	software	6
789	createUnit	createUnit	LEaP command to create a new UNIT object	software	7
790	desc	desc	LEaP command to print a description of an object	software	24
791	groupSelectedAtoms	groupSelectedAtoms	LEaP command to create a named group of selected atoms	software	4
792	help	help	LEaP command to display help information	software	147
793	list	list	LEaP command to list all currently defined variables	software	415
794	loadOff	loadOff	LEaP command to load an OFF library file	software	9
795	loadPdbUsingSeq	loadPdbUsingSeq	LEaP command to load a PDB file using a user-defined sequence	software	6
796	logFile	logFile	LEaP command to specify a file for logging all input and output	software	12
797	measureGeom	measureGeom	LEaP command to measure distance, angle, or torsion	software	5

798	quit	quit	LEaP command to exit the program	software	22
799	remove	remove	LEaP command to remove an object from a container	software	49
800	saveMol2	saveMol2	LEaP command to save a unit in Tripos mol2 format	software	3
801	saveOff	saveOff	LEaP command to save objects to an OFF library file	software	7
802	set	set	LEaP command to set default parameters or properties of objects	software	1215
803	setBox	setBox	LEaP command to create a periodic box around a solute	software	6
804	solvateCap	solvateCap	LEaP command to create a spherical solvent cap around a solute	software	6
805	solvateShell	solvateShell	LEaP command to add a solvent shell of a specified thickness around a solute	software	5
806	source	source	LEaP command to execute commands from a script file	software	115
807	transform	transform	LEaP command to apply a symmetry transformation matrix to atoms	software	12
808	translate	translate	LEaP command to translate atoms by a given vector	software	18
809	verbosity	verbosity	LEaP command to set the level of output messages	software	49
810	zMatrix	zMatrix	LEaP command to define Cartesian coordinates using internal coordinates	software	11
811	GLYCAM-Web	GLYCAM-Web	A web server for building carbohydrate and glycoprotein structures	software|data source	4
812	GlcpNAc-OH	GlcpNAc-(1–4)-β-d-	Chemical structure of a trisaccharide core common in N-glycans.	chemical entity|model	0
813	β-d-mannopyranose	β-d-mannopyranose	A specific mannose sugar isomer, often a branch point.	chemical entity	0
814	ROH	ROH	Residue name for a reducing-end hydroxyl group in GLYCAM.	identifier|chemical entity	9
815	4YB	4YB	Residue name for β-D-GlcpNAc in GLYCAM nomenclature.	identifier|chemical entity	21
816	VMB	VMB	Residue name for a 3,6-branched β-D-mannopyranose in GLYCAM.	identifier|chemical entity	11
817	0MA	0MA	Residue name for α-D-Manp in GLYCAM nomenclature.	identifier|chemical entity	17
818	set glycan tail	set glycan tail	LEaP command to define the attachment point for subsequent residues.	software|process	6
819	Man-9	Man-9	A specific high-mannose N-glycan with nine mannose residues.	chemical entity	1
820	Consortium for Functional Glycomics	Functional Glycomics	An organization providing resources and standards for glycan representation.	data source|model	2
821	VMA	VMA	Residue name for a 3,6-branched α-D-Manp residue.	identifier|chemical entity	2
822	2MA	2MA	Residue name for a 2-linked α-D-Manp residue.	identifier|chemical entity	4
823	DMPC	DMPC	1,2-dimyristoyl-sn-glycero-3-phosphocholine, a common model lipid.	chemical entity	9
824	CHO	CHO	Fragment name for the choline head group in GLYCAM lipids.	identifier|chemical entity	5
825	PGL	PGL	Fragment name for the phospho-glycerol group in GLYCAM lipids.	identifier|chemical entity	11
826	MYR	MYR	Fragment name for the sn-1 chain myristic acid tail.	identifier|chemical entity	3
827	MY2	MY2	Fragment name for the sn-2 chain myristic acid tail.	identifier|chemical entity	4
828	Glycoprotein	Glycoprotein	A protein with one or more covalently attached glycans.	chemical entity	10
829	N-linked glycosylation	N-linked glycosylation	Attachment of a glycan to an asparagine (Asn) residue.	process|model	0
830	O-linked glycosylation	O-linked glycosylation	Attachment of a glycan to a serine (Ser) or threonine (Thr) residue.	process|model	0
831	Ribonuclease A	Ribonuclease A	A protein used as an example for glycosylation.	chemical entity	1
832	PDBID	PDBID	Protein Data Bank identifier, a unique code for structures.	identifier	4
833	3RN3	3RN3	PDBID for bovine ribonuclease A.	identifier|data source	3
834	Disulfide bond	SSBOND	A covalent bond between two cysteine residues.	chemical entity|model	4
835	OLS	OLS	Modified serine residue name for O-linkages in Amber.	identifier|chemical entity	1

836	OLT	OLT	Modified threonine residue name for O-linkages in Amber.	identifier|chemical entity	1
837	OLP	OLP	Modified hydroxyproline residue name for O-linkages in Amber.	identifier|chemical entity	1
838	NLN	NLN	Modified asparagine residue name for N-linkages in Amber.	identifier|chemical entity	2
839	Glycoprotein Builder	Glycoprotein Builder	A web tool at glycam.org for building glycoprotein models.	software|data source	2
840	Solvate.sh	Solvate.sh	An AmberTools script to solvate a system with a target number of waters.	software|process	4
841	parmtop	parmtop	Amber parameter-topology file containing system-specific force field information.	data format	27
842	crd	crd	Amber coordinate file format.	data format	78
843	rst7	rst7	Amber restart coordinate file format.	data format	30
844	dat file	.dat	Standard Amber parameter file containing force field definitions.	data format	33
845	Bond Stretching	Σ k_b(r-r_0)^2	Energy term for the vibration of covalent bonds.	model	7
846	k_b	k_b	Force constant for the bond stretching term.	measure|model	0
847	r_0	r_0	Equilibrium bond length for the bond stretching term.	measure|model	0
848	Angle Bending	Σ k_θ(θ-θ_0)^2	Energy term for the bending of angles between three atoms.	model	5
849	k_θ	k_θ	Force constant for the angle bending term.	measure|model	0
850	θ_0	θ_0	Equilibrium angle value for the angle bending term.	measure|model	0
851	Dihedral Term	Σ V_n[1+cos(nφ-γ)]	Energy term for rotation around a central bond (torsion).	model	3
852	V_n	V_n	Barrier height for the dihedral term.	measure|model	0
853	n	n	Periodicity of the dihedral term.	measure|model	652
854	1-4 Interaction	1-4 Interaction	Non-bonded interaction between atoms separated by three bonds.	model	1
855	SCEE	SCEE	Scaling factor for 1-4 electrostatic interactions.	measure|model	14
856	SCNB	SCNB	Scaling factor for 1-4 van der Waals interactions.	measure|model	13
857	Out-of-Plane Term	Out-of-Plane Term	An improper torsion used to maintain planarity.	model	0
858	A_ij	A_ij	The repulsive (R^-12) coefficient in the Lennard-Jones potential.	measure|model	0
859	B_ij	B_ij	The attractive (R^-6) coefficient in the Lennard-Jones potential.	measure|model	0
860	R_min	R_min	Distance at the minimum of the Lennard-Jones potential well.	measure|model	0
861	ε (epsilon)	ε	Depth of the Lennard-Jones potential well.	measure|model	2
862	σ (sigma)	σ	The finite distance at which the Lennard-Jones potential is zero.	measure|model	0
863	Lorentz-Berthelot mixing rules	rules	Rules to combine Lennard-Jones parameters for different atom types.	method|model	1
864	Partial Charge	q_i	A fixed point charge assigned to an atom in a molecule.	measure|state	8
865	addAtomicNumber	addAtomicNumber	ParmEd command to add atomic numbers to a topology file.	software|process	3
866	addDihedral	addDihedral	ParmEd command to add a new dihedral term.	software|process	3
867	addExclusions	addExclusions	ParmEd command to add non-bonded interaction exclusions.	software|process	3
868	addLJType	addLJType	ParmEd command to create a new Lennard-Jones atom type.	software|process	11
869	addPDB	addPDB	ParmEd command to add PDB information to the topology file.	software|process	7
870	chamber	chamber	A ParmEd tool to convert CHARMM files to Amber format.	software|process	28
871	Residue Topology File	RTF	CHARMM file defining residue connectivity and atom types.	data format	18
872	Parameter File	PAR	CHARMM file containing force field parameters.	data format	58
873	Protein Structure File	PSF	CHARMM file defining the specific molecular system's topology.	data format	19

874	NBFIX	NBFIX	CHARMM term for modifying specific pairwise non-bonded interactions.	model|method	2
875	changeLJPair	changeLJPair	ParmEd command to modify a specific Lennard-Jones pairwise interaction.	software|process	7
876	changeRadii	changeRadii	ParmEd command to change the set of Generalized Born radii.	software|process	5
877	checkValidity	checkValidity	ParmEd command to perform consistency checks on a topology file.	software|process	6
878	energy	energy	ParmEd command to compute the potential energy of a system.	software|process	1151
879	gromber	gromber	ParmEd command to convert GROMACS topology files to Amber format.	software|process	4
880	GROMACS	GROMACS	A widely used molecular dynamics simulation package.	software	25
881	interpolate	interpolate	ParmEd command to create intermediate topologies for free energy calculations.	software|process	12
882	loadCoordinates	loadCoordinates	ParmEd command to load coordinates from various file formats.	software|process	3
883	minimize	minimize	ParmEd command to perform energy minimization, often using OpenMM.	software|process	32
884	OpenMM	OpenMM	A high-performance, open-source toolkit for molecular simulation.	software|library	40
885	outCIF	outCIF	ParmEd command to write a PDBx/mmCIF file.	software|process	3
886	PDBx/mmCIF	PDBx/mmCIF	The standard archive format for macromolecular structures.	data format	7
887	parmout	parmout	ParmEd command to specify the final output topology file.	software|process	9
888	strip	strip	ParmEd command to remove a selection of atoms from the system.	software|process	19
889	writeFrcmod	writeFrcmod	ParmEd command to generate a frcmod file from a topology.	software|process	3
890	writeOFF	writeOFF	ParmEd command to write an Amber OFF library file.	software|process	3
891	AmberParm	AmberParm	A Python class in ParmEd representing an Amber topology file.	software|data format	15
892	ParmedTools	ParmedTools	A Python package containing the actions available in ParmEd.	software	1
893	GAFF	GAFF	General AMBER Force Field for small organic molecules.	model|data source	62
894	gaff.dat	gaff.dat	The parameter file for the General AMBER Force Field.	data source|data format	12
895	HF/6-31G* RESP	HF/6-31G* RESP	A quantum mechanical method for calculating atomic charges.	method|model	4
896	ABCG2	ABCG2	An atom-bond charge correction model at the G2 level.	method|model	15
897	MP2/6-31G*	MP2/6-31G*	A level of theory for ab initio quantum calculations.	method|model	2
898	Cambridge Structural Database	Database	A repository for small-molecule crystal structures.	data source	1
899	PARMSCAN	PARMSCAN	A software package used to optimize torsional angle parameters.	software	1
900	parmchk2	parmchk2	A program to check for and generate missing force field parameters.	software	14
901	divcon	divcon	A quantum chemistry program.	software	4
902	atomtype (program)	atomtype	A program within Antechamber that assigns atom types.	software|process	10
903	am1bcc (program)	am1bcc	A program within Antechamber that calculates AM1-BCC charges.	software|process	7
904	bondtype (program)	bondtype	A program within Antechamber that assigns detailed bond types.	software|process	12
905	espgen (program)	espgen	A program within Antechamber to extract electrostatic potential data.	software|process	20
906	respgen (program)	respgen	A program within Antechamber to generate input for RESP fitting.	software|process	11
907	prepgen	prepgen	A program within Antechamber to generate Amber prep input files.	software|process	10
908	ac file format	ac	Antechamber file format containing molecular structure and properties.	data format	62
909	AMBER PREP (int)	prepi	Amber preparatory file with internal coordinates.	data format	16
910	AMBER PREP (car)	prepc	Amber preparatory file with Cartesian coordinates.	data format	9
911	Gaussian Z-Matrix	gzmat	Gaussian input file format using Z-matrix coordinates.	data format	4

912	Gaussian Cartesian	gcrt	Gaussian input file format using Cartesian coordinates.	data format	8
913	Gaussian Output	gout	Output file from a Gaussian calculation.	data format	22
914	Gaussian ESP	gesp	Gaussian file containing electrostatic potential grid data.	data format	14
915	Component cif	ccif	Crystallographic Information File for a chemical component.	data format	3
916	CM1 charge method	cm1	Charge Model 1, a semi-empirical charge model.	method|model	2
917	CM2 charge method	cm2	Charge Model 2, an improved semi-empirical charge model.	method|model	3
918	ESP (Kollman) charge method	esp	Electrostatic potential fitting method developed by Kollman's group.	method|model	57
919	Mulliken charge method	mul	A method for calculating atomic charges from quantum calculations.	method|model	1
920	Gasteiger charge method	gas	An empirical method for calculating partial atomic charges.	method|model	36
921	charge equilibration	charge equilibration	Process of forcing charges of symmetrically equivalent atoms to be equal.	process|method	5
922	PARMCHK.DAT	PARMCHK.DAT	Antechamber data file with atom type similarity scores for parameter checking.	data source	3
923	ATCOR.DAT	ATCOR.DAT	Antechamber data file listing replaceable general atom types.	data source	1
924	similarity score	similarity score	A metric measuring the similarity between atom types for parameter estimation.	measure	1
925	leaprc.gaff	leaprc.gaff	LEaP script that loads the GAFF force field.	data source|software	1
926	acdoctor	acdoctor	A program to diagnose potential problems in molecular input files.	software	17
927	CONNECT.TPL	CONNECT.TPL	A template file defining standard connectivity for antechamber.	data source	1
928	ATOMTYPE_AMBER.DEF	F	Definition file for standard AMBER atom types.	data source	1
929	ATOMTYPE_GFF.DEF	ATOMTYPE_GFF.DEF	Definition file for GAFF atom types.	data source	2
930	BCCPARM.DAT	BCCPARM.DAT	Parameter file containing bond charge corrections for the AM1-BCC method.	data source	1
931	parmcal	parmcal	An interactive program to calculate bond and angle parameters.	software	4
932	residuegen	residuegen	A program to facilitate the generation of modified residue topologies.	software|process	8
933	match	match	A program to perform least-squares fitting between two molecules.	software|process	75
934	match_atomname	match_atomname	A program to match atom names between a reference and input file.	software|process	7
935	paramfit	paramfit	A program to fit force field parameters to quantum mechanical data.	software	67
936	Job Control File	Job_Control.in	The main input file for the paramfit program.	data format	31
937	RUNTYPE	RUNTYPE	paramfit variable specifying the type of job to perform.	identifier	13
938	CREATE_INPUT	CREATE_INPUT	A paramfit RUNTYPE for creating quantum package input files.	state|process	5
939	SET_PARAMS	SET_PARAMS	A paramfit RUNTYPE for interactively specifying parameters to be fit.	state|process	4
940	FIT	FIT	A paramfit RUNTYPE for conducting the parameter fitting process.	state|process	168
941	QMHEADER	QMHEADER	A file containing header information for quantum calculation input files.	data source	3
942	QMFILEFORMAT	QMFILEFORMAT	paramfit variable specifying the quantum package file format.	identifier	2
943	ALGORITHM	ALGORITHM	paramfit variable specifying the minimization algorithm to use.	identifier	182
944	Genetic Algorithm	GENETIC	An optimization algorithm that mimics natural selection.	algorithm|method	16
945	Simplex Algorithm	SIMPLEX	A local minimization algorithm based on a geometric simplex.	algorithm|method	22
946	FUNC_TO_FIT	FUNC_TO_FIT	paramfit variable specifying the objective function for fitting.	identifier	2
947	K (energy offset)	K	A constant representing the intrinsic energy difference between QM and MM.	measure|model	247
948	Bounds Checking	CHECK_BOUNDS	A process in paramfit to ensure fitted parameters are physically reasonable.	process|method	7
949	&fitq	&fitq	The mdgx namelist for controlling electrostatic potential fitting.	identifier	4

950	RespPhi	RespPhi	mdgx keyword to specify an electrostatic potential file for RESP fitting.	identifier	4
951	IPolQPhi	IPolQPhi	mdgx keyword to specify electrostatic potential files for IPolQ fitting.	identifier	1
952	Virtual Site	ExtraPoint	A massless point whose position is defined by massive atoms.	model	24
953	&ipolq	&ipolq	The mdgx namelist for controlling IPolQ charge development.	identifier	4
954	Solvent Reaction Field Potential	SRFP	The electrostatic potential generated by the time-averaged solvent charge density.	measure|model	15
955	&rule	&rule	The mdgx namelist for defining virtual site construction rules.	identifier	4
956	Frame Style	FrameStyle	A specific geometric method for constructing a virtual site.	model|identifier	2
957	&param	&param	The mdgx namelist for controlling bonded parameter fitting.	identifier	4
958	&configs	&configs	The mdgx namelist for controlling configuration sampling.	identifier	8
959	l/r-RESPA	l/r-RESPA	A multiple time-stepping integration scheme.	algorithm|method	2
960	&pptd	&pptd	The mdgx namelist for controlling the peptide multi-simulator on GPUs.	identifier	3
961	MCPB.py	MCPB.py	A Python tool for building parameters for metal centers.	software	24
962	Bonded model (metal)	bonded model	A model treating metal ions as covalently bonded to their ligands.	model	5
963	Nonbonded model (metal)	nonbonded model	A model treating metal ions purely with non-bonded interactions.	model	16
964	IPMach.py	IPMach.py	A Python tool for automated ion parameterization.	software	7
965	PdbSearcher.py	PdbSearcher.py	A Python tool to search for metal centers in PDB files.	software	6
966	OptC4.py	OptC4.py	A program to optimize C4 terms for the 12-6-4 potential.	software	5
967	amb2chm_par.py	amb2chm_par.py	A script to convert Amber dat/frcmod to a CHARMM parameter file.	software	5
968	ion_paraset	ion_paraset	MCPB.py variable for the ion parameter set in the nonbonded model.	identifier	1
969	Hydration Free Energy	HFE	The free energy change when an ion is transferred from vacuum to water.	measure	35
970	Ion-Oxygen Distance	IOD	The average distance between an ion and oxygen atoms in its first solvation shell.	measure	30
971	12-6-4 LJ-type model	12-6-4 LJ-type model	A nonbonded model including an ion-induced dipole (C4) term.	model	4
972	Empirical method (MCPB.py)	Empirical method	A method in MCPB.py to generate parameters without QM calculations.	method|model	1
973	fluctuating charge model	fluctuating charge model	A charge model where atomic charges can vary in response to the environment.	model|method	4
974	Applequist scheme	Applequist	A method for calculating induced dipoles without damping.	model|method	5
975	Tinker-exponential damping	Tinker-exponential	A specific functional form for damping electrostatic interactions.	model|method	3
976	mdinfo	mdinfo	An output file containing the most recent energy information from sander.	data format	17
977	refc	refc	An input file containing reference coordinates for restraints.	data format	5
978	mdcrd	mdcrd	An output file containing coordinate trajectory frames.	data format	58
979	inptraj	inptraj	An input trajectory file for post-processing with sander.	data format	6
980	mdvel	mdvel	An output file containing velocity trajectory frames.	data format	7
981	mdfrc	mdfrc	An output file containing force trajectory frames.	data format	3
982	mden	mden	An output file containing detailed energy data over a trajectory.	data format	8
983	evbin	evbin	An input file for Empirical Valence Bond (EVB) potentials.	data format	3
984	ntxo	ntxo	sander variable controlling the format of the output restart file.	identifier	6
985	iwrap	iwrap	sander flag to wrap coordinates into the primary periodic box.	identifier	12
986	ntwv	ntwv	sander variable for the frequency of writing velocities to the trajectory.	identifier	10
987	ntwf	ntwf	sander variable for the frequency of writing forces to the trajectory.	identifier	8

988	ntwe	ntwe	sander variable for the frequency of writing energies to the mden file.	identifier	8
989	ioutfm	ioutfm	sander variable controlling the format (ASCII/NetCDF) of trajectory files.	identifier	17
990	ntwprt	ntwprt	sander variable specifying the number of atoms to write to trajectories.	identifier	6
991	ntr	ntr	sander flag to apply Cartesian restraints to specified atoms.	identifier	19
992	restraint_wt	restraint_wt	The force constant for Cartesian restraints.	measure	4
993	restraintmask	restraintmask	An Amber mask string specifying atoms to be restrained.	identifier	6
994	bellymask	bellymask	An Amber mask string specifying atoms to be moved in a belly simulation.	identifier	5
995	ncyc	ncyc	The number of steepest descent steps before switching to conjugate gradient.	identifier	7
996	ntmin	ntmin	etc.).	identifier	13
997	dx0	dx0	The initial step length for energy minimization.	measure	3
998	nstlim	nstlim	The total number of molecular dynamics steps to perform.	identifier	78
999	nscm	nscm	The frequency for removing center-of-mass motion.	identifier	9
1000	dt	dt	The time step for molecular dynamics integration in picoseconds.	measure|unit	58
1001	Hydrogen Mass Repartitioning	HMR	A method to increase hydrogen mass to allow for larger timesteps.	method	11
1002	ntt	ntt	sander flag to select the thermostat for temperature regulation.	identifier	69
1003	Andersen thermostat	Andersen thermostat	A temperature control method using stochastic collisions.	algorithm|method	12
1004	Langevin dynamics	Langevin dynamics	forces.	algorithm|method	28
1005	Nose-Hoover chain	Nose-Hoover chain	A deterministic method for canonical ensemble (NVT) simulations.	algorithm|method	3
1006	Bussi thermostat	Bussi thermostat	A stochastic velocity rescaling thermostat that generates a canonical distribution.	algorithm|method	1
1007	tempi	tempi	The initial temperature for velocity assignment in Kelvin.	measure|unit	28
1008	ig	ig	The seed for the pseudo-random number generator.	identifier	35
1009	tautp	tautp	The time constant for the Berendsen thermostat in picoseconds.	measure|unit	15
1010	gamma_ln	gamma_ln	The collision frequency for Langevin dynamics in ps^-1.	measure|unit	34
1011	vlimit	vlimit	A velocity limit to prevent simulation instabilities.	measure	7
1012	ntp	ntp	sander flag to select the barostat for pressure regulation.	identifier	27
1013	isotropic position scaling	isotropic position scaling	A pressure coupling method where the box scales uniformly in all directions.	method	1
1014	anisotropic position scaling	scaling	A pressure coupling method where box dimensions scale independently.	method	0
1015	Berendsen barostat	Berendsen barostat	A weak-coupling method for pressure control.	algorithm|method	2
1016	Monte Carlo barostat	Monte Carlo barostat	A pressure control method using Monte Carlo volume moves.	algorithm|method	10
1017	pres0	pres0	The target pressure for the simulation in bars.	measure|unit	3
1018	comp	comp	The compressibility of the system, used by the Berendsen barostat.	measure	2
1019	modified Seminario method	msem	A modified version of the Seminario method for force constants.	method|algorithm	3
1020	RESP-perm-v	RESP-perm-v	A RESP-perm model that includes virtual permanent dipoles.	model|method	7
1021	SHAKE	SHAKE	An algorithm to constrain bond lengths, allowing larger time steps.	algorithm|method	79
1022	middle scheme	middle scheme	A unified framework for developing efficient thermostatting algorithms.	method|algorithm	10
1023	LFMiddle	LFMiddle	The leapfrog algorithm implementation within the 'middle' scheme.	algorithm|method	18
1024	SETTLE	SETTLE	An analytical algorithm for constraining rigid water molecules.	algorithm|method	6
1025	ischeme	ischeme	sander flag for choosing the integration scheme (e.g., middle scheme).	identifier	11

1026	ithermostat	ithermostat	sander flag for choosing the thermostat in the 'middle' scheme.	identifier	14
1027	therm_par	therm_par	The primary parameter (e.g., friction) for a 'middle' scheme thermostat.	measure	13
1028	Path Integral Molecular Dynamics	PIMD	A simulation method to include nuclear quantum effects.	method|process	29
1029	sander_input	sander_input	A data structure in the sander API for providing input parameters.	data format|software	45
1030	taup	taup	Pressure relaxation time constant for the Berendsen barostat.	measure|unit	3
1031	constant surface tension	constant surface tension	A simulation condition used for systems with interfaces, like membranes.	state|process	10
1032	csurften	csurften	sander flag to enable constant surface tension dynamics.	identifier	3
1033	gamma_ten	gamma_ten	The target surface tension value in dyne/cm.	measure|unit	2
1034	ninterface	ninterface	The number of interfaces in the system for surface tension calculations.	measure	2
1035	tol	tol	The geometric tolerance for the SHAKE algorithm.	measure	33
1036	noshakemask	noshakemask	An Amber mask to specify atoms excluded from SHAKE constraints.	identifier	9
1037	Ornstein-Uhlenbeck process	process	The stochastic process underlying Langevin dynamics.	model|method	0
1038	VVMiddle	VVMiddle	The velocity-Verlet algorithm implementation within the 'middle' scheme.	algorithm|method	6
1039	water cap	water cap	A spherical portion of explicit water centered on a solute.	model	1
1040	ivcap	ivcap	sander flag to control the water cap option.	identifier	4
1041	fcap	fcap	The force constant for the water cap restraint potential.	measure	2
1042	fswitch	fswitch	sander flag to enable force switching for nonbonded interactions.	identifier	7
1043	nsnb	nsnb	The frequency for updating the nonbonded pair list.	measure	7
1044	ipol	ipol	sander flag to enable a polarizable force field.	identifier	12
1045	ipgm	ipgm	sander flag to enable the polarizable Gaussian Multipole (pGM) force field.	identifier	4
1046	ievb	ievb	sander flag to enable the Empirical Valence Bond (EVB) method.	identifier	3
1047	efx	efx	The x-component of an applied external electric field.	measure	8
1048	mcwat	mcwat	sander flag to enable Monte Carlo water equilibrium sampling.	identifier	3
1049	ntwd	ntwd	sander flag to enable Thermodynamic Integration (TI) Free Energy Decomposition.	identifier	2
1050	ramdboost	ramdboost	The acceleration boost strength for Random Acceleration Molecular Dynamics (RAMD).	measure	3
1051	reweight	reweight	sander flag to re-evaluate energies/forces on an existing trajectory.	identifier	7
1052	midpoint	midpoint	sander flag to enable midpoint optimizations (3D spatial decomposition).	identifier	18
1053	&ewald	&ewald	The namelist in sander for controlling PME and related parameters.	identifier	14
1054	nfft1	nfft1	The size of the PME charge grid in the x-dimension.	measure	15
1055	skinnb	skinnb	The width of the buffer region for the nonbonded pair list.	measure	6
1056	frameon	frameon	sander flag controlling the treatment of extra points.	identifier	4
1057	indmeth	indmeth	sander flag specifying the method for calculating induced dipoles.	identifier	11
1058	Car-Parrinello scheme	Car-Parrinello scheme	A method where induced dipoles are treated as dynamic variables with mass.	algorithm|method	0
1059	&dipoles	&dipoles	The namelist in sander for enabling the printing of dipole moments.	identifier	1
1060	profile_mpi	profile_mpi	sander flag to control detailed timing output for parallel runs.	identifier	3
1061	&pol_gauss	&pol_gauss	The namelist in sander for controlling the pGM force field.	identifier	2
1062	ee_dsum_cut	ee_dsum_cut	The direct sum cutoff for pGM electrostatic calculations.	measure	6
1063	dipole_scf_tol	dipole_scf_tol	The convergence criterion for the induced dipole self-consistent field calculation.	measure	5

1064	&wt	&wt	The namelist in sander for specifying time-dependent changes to simulation parameters.	identifier	22
1065	&debugf	&debugf	The namelist in sander for accessing debugging options.	identifier	11
1066	groupfile	groupfile	An input file for multisander specifying the command line for each replica.	data format	100
1067	sander.APBS	sander.APBS	A version of sander compiled with the APBS Poisson-Boltzmann solver.	software	10
1068	pysander	pysander	A shorthand term for using the sander API within a Python script.	software|library	3
1069	Fast Water Update Algorithm	jfastw	Selector for a fast water update algorithm.	algorithm|method	10
1070	QM/MM Input Options	qmmm_input_options	Data structure containing settings for QM/MM simulations.	data format|model	25
1071	SCF Error Convergence	errconv	SCF tolerance on the maximum error matrix value.	measure|algorithm	5
1072	DFTB Electronic Temperature Step	dftb_telec_step	Step size for reducing electronic temperature in DFTB calculations.	measure|method	2
1073	Fock Matrix Prediction Prefactor 1	fockp_d1	First prefactor for Fock matrix prediction.	measure|algorithm	2
1074	Fock Matrix Prediction Prefactor 2	fockp_d2	Second prefactor for Fock matrix prediction.	measure|algorithm	2
1075	Fock Matrix Prediction Prefactor 3	fockp_d3	Third prefactor for Fock matrix prediction.	measure|algorithm	2
1076	Fock Matrix Prediction Prefactor 4	fockp_d4	Fourth prefactor for Fock matrix prediction.	measure|algorithm	2
1077	SCF Damping Factor	damp	Damping factor used in Self-Consistent Field calculations.	measure|algorithm	8
1078	Debye Salt Concentration Parameter	kappa	Parameter related to Debye salt concentration for GB models.	measure|model	6
1079	Pseudo-diagonalization Criterion	pseudo_diag_criteria	Criterion for performing pseudo-diagonalization of the Fock matrix.	measure|algorithm	5
1080	Minimum Heavy-Atom Mass	min_heavy_mass	Minimum mass for an atom to be considered a heavy-atom.	measure|unit	4
1081	QM/MM Switch Upper Distance	r_switch_hi	Distance at which the QM/MM switching function goes to zero.	measure|unit	8
1082	QM/MM Switch Lower Distance	r_switch_lo	Distance at which the QM/MM switching function turns on.	measure|unit	6
1083	DIIS Matrices	ndiis_matrices	Number of error vectors for the DIIS convergence algorithm.	measure|algorithm	3
1084	QM-QM Derivative Calculation	qmqmdx	Controls whether QM-QM derivatives are computed analytically or pseudo-numerically.	method|algorithm	6
1085	Peptide Linkage Correction	peptide_corr	Flag to apply a MM correction to peptide linkages.	method|model	4
1086	QM-MM In-Core Storage	qmmmrij_incore	Flag to store QM-MM pairs and related equations in memory.	method|process	2
1087	QM-QM In-Core Storage	qmqm_erep_incore	Flag to store QM-QM 1-electron repulsion integrals in memory.	method|process	2
1088	Pseudo-diagonalization	pseudo_diag	Flag to allow the use of pseudo-diagonalization of the Fock matrix.	algorithm|method	9
1089	QM Ewald Treatment	qm_ewald	Specifies how long-range electrostatics for the QM region are treated.	method|algorithm	12
1090	QM Particle Mesh Ewald	qm_pme	Flag to use PME for QM long-range electrostatic interactions.	method|algorithm	5
1091	K-space Vectors (X)	kmaxqx	Number of K-space vectors in the X-dimension for Ewald/PME.	measure|algorithm	4
1092	K-space Vectors (Y)	kmaxqy	Number of K-space vectors in the Y-dimension for Ewald/PME.	measure|algorithm	2
1093	K-space Vectors (Z)	kmaxqz	Number of K-space vectors in the Z-dimension for Ewald/PME.	measure|algorithm	2
1094	Maximum K-squared	ksqmaxsq	Maximum K^2 values for spherical cutoff in reciprocal space.	measure|algorithm	2
1095	Tight Density Convergence	tight_p_conv	Controls the tightness of the density matrix convergence criteria.	measure|algorithm	4
1096	Diagonalization Routine	diag_routine	Selects the routine to diagonalize the Fock matrix.	algorithm|method	13
1097	Density Prediction	density_predict	Flag to use the density matrix from the previous step.	method|algorithm	2
1098	Fock Matrix Prediction	fock_predict	Flag to attempt prediction of the Fock matrix.	method|algorithm	6
1099	Hot Spot Adaptive Calculation	hot_spot	Activates adaptive calculation with force smoothing in buffer region.	method|algorithm	4
1100	Core QM Atom Indices	core_iqmatoms	List of atom indices for the core QM/MM region.	identifier|data format	3
1101	Buffer QM Atom Indices	buffer_iqmatoms	List of atom indices for the buffer QM/MM region.	identifier|data format	3

1102	Center Region Mask	centermask	Amber selection mask that defines the center region.	identifier|data format	6
1103	Potential Energy Terms	pot_ene	Data structure containing components of the potential energy.	data format	7
1104	Total Potential Energy	tot	The total potential energy of the system.	measure	17
1105	Dihedral Energy	dihedral	The energy contribution from valence torsions.	measure	152
1106	1-4 Van der Waals Energy	vdw_14	The energy contribution from 1-4 van der Waals interactions.	measure	2
1107	1-4 Electrostatic Energy	elec_14	The energy contribution from 1-4 electrostatic interactions.	measure	2
1108	Restraint Energy	constraint	The total restraint energy from NMR or positional restraints.	measure	77
1109	Polarization Energy	polar	The polarization energy if using a polarizable force field.	measure	89
1110	10-12 H-bond Energy	hbond	The 10-12 contribution to the total energy.	measure	3
1111	Surface Area Energy	surf	The non-polar solvation free energy contribution from GB/PB.	measure	3
1112	Self-Consistent Field Energy	scf	The QM energy contribution to the total energy.	measure	90
1113	Improper Torsion Energy	imp	The improper torsion contribution to the total energy (CHARMM).	measure	3
1114	Electron Density Map Restraint Energy	emap	Restraint energy from violations to an electron density map.	measure	34
1115	Charge Transfer Energy	ct	The charge transfer energy contribution.	measure	10
1116	Accelerated MD Boost Energy	amd_boost	The boosting energy from Accelerated Molecular Dynamics.	measure	1
1117	Gas-phase/GB Sander Input	gas_sander_input	Function to initialize sander input for gas-phase or GB calculations.	process|software	9
1118	PME Sander Input	pme_sander_input	Function to initialize sander input for PME calculations.	process|software	8
1119	QM Sander Input	qm_sander_input	Function to initialize QM/MM input options with defaults.	process|software	7
1120	Sander Setup	sander_setup	Function to set up the sander API for calculations.	process|software	9
1121	Set Positions	set_positions	Function to set the active atomic coordinates in the API.	process|software	4
1122	Set Box	set_box	Function to set the unit cell dimensions in the API.	process|software	4
1123	Get Sander Atom Count	sander_natom	Function that returns the number of atoms in the system.	process|software	9
1124	Get Positions	get_positions	Function to retrieve the current atomic coordinates from the API.	process|software	4
1125	Get Inpcrd Atom Count	get_inpcrd_natom	Function to read the number of atoms from an inpcrd file.	process|software	12
1126	Read Inpcrd File	read_inpcrd_file	Function to read coordinates and box from an inpcrd file.	process|software	9
1127	Check Setup Status	is_setup	Function that returns whether a system is currently set up.	process|software	4
1128	Calculate Energy and Forces	energy_forces	Function to compute the energy and forces for the current coordinates.	process|software	13
1129	Sander Cleanup	sander_cleanup	Function to clear internal memory allocated by the sander API.	process|software	10
1130	Isotropic Periodic Sums	Isotropic Periodic Sums	A method for handling long-range interactions in non-periodic systems.	method|algorithm	1
1131	Middle Thermostat Scheme	middle thermostat	A specific thermostatting algorithm for temperature control.	algorithm|method	2
1132	Adaptively Biased MD	Adaptively biased MD	An enhanced sampling technique that applies a bias to the system.	method|algorithm	2
1133	Semi-Isotropic Pressure Scaling	scaling	A pressure coupling scheme allowing different scaling in xy and z dimensions.	method|algorithm	1
1134	Non-bonded Flag	nbflag	Flag to control non-bonded list update scheduling.	method|process	8
1135	Direct Sum Coulomb Method	eedmeth	Method for the direct space part of the Ewald sum.	method|algorithm	6
1136	mdout Flush Interval	mdout_flush_interval	Controls the time interval for flushing the main output file.	measure|process	2
1137	mdinfo Flush Interval	mdinfo_flush_interval	Controls the time interval for flushing the info file.	measure|process	3
1138	Electrostatic Cutoff	es_cutoff	Cutoff distance for direct space electrostatic interactions in PME.	measure|unit	6
1139	Van der Waals Cutoff	vdw_cutoff	Cutoff distance for van der Waals interactions.	measure|unit	6

1140	Intermolecular Bonds Flag	no_intermolecular_bonds	Controls how molecules connected by bonds are treated for pressure calculations.	method|process	2
1141	Energy Averaging Sampling	ene_avg_sampling	Frequency of energy sampling for running averages.	measure|process	2
1142	Axis Optimization	use_axis_opt	Flag to control reorientation of unit cell axes for performance.	process|algorithm	6
1143	FFT Grids per Angstrom	fft_grids_per_ang	Sets the density of the Fast Fourier Transform grid.	measure|algorithm	1
1144	FFT Grid Dimensions	nfft1, nfft2, nfft3	The dimensions of the Fast Fourier Transform grid.	measure|algorithm	1
1145	Multiple Time-Stepping Algorithm	respa	An algorithm that uses different time steps for different interactions.	algorithm|method	17
1146	PMEMD GPU MPI Version	pmemd.cuda.MPI	Multi-GPU parallel version of the pmemd.cuda program.	software	13
1147	SPFP Precision Model	SPFP	Hybrid Single/Fixed Precision model for GPU calculations.	model|method	7
1148	DPFP Precision Model	DPFP	Double Precision/Fixed Precision model for GPU calculations.	model|method	2
1149	SPXP Precision Model	SPXP	Experimental Single/Mixed Precision model for GPU calculations.	model|method	1
1150	Kepler GPU Architecture	Kepler architecture	An NVIDIA GPU microarchitecture generation.	software	1
1151	Volta GPU Architecture	Volta architecture	An NVIDIA GPU microarchitecture generation.	software	1
1152	PCI-Express	PCI-E	A standard for high-speed computer expansion card connections.	software	3
1153	Peer-to-Peer Communication	communication	Direct data transfer between GPUs, bypassing the CPU.	process|method	2
1154	CUDA Visible Devices	S	An environment variable to control which GPUs are visible to an application.	identifier|software	12
1155	Barostat	barostat	An algorithm used to control pressure in a simulation.	algorithm|method	24
1156	Anderson Thermostat	Anderson Thermostat	A stochastic algorithm for temperature control in the canonical ensemble.	algorithm|method	2
1157	Langevin Thermostat	Langevin Thermostat	A stochastic thermostat that mimics solvent effects.	algorithm|method	22
1158	Net Force Removal	netfrc	Flag to calculate and remove the net system force during PME.	method|process	10
1159	MVAPICH2-GDR	MVAPICH2-GDR	An MPI library supporting GPU-Direct communication for high performance.	software	3
1160	Error-Correcting Code Memory	ECC	A type of computer memory that can detect and correct data corruption.	state	6
1161	NVIDIA NCCL	NCCL	NVIDIA Collective Communications Library for multi-GPU communication primitives.	software	21
1162	Amber Mask	Amber Mask	A text-based notation for selecting atoms and residues in Amber.	identifier|data format	19
1163	NAB Atom Expression	NAB atom expressions	A selection syntax used in applications built with NAB.	identifier|data format	1
1164	GROUP Specification	GROUP Specification	A legacy format for defining groups of atoms in sander and pmemd.	identifier|data format	1
1165	ambmask utility	ambmask	An Amber utility to test and apply atom/residue selection masks.	software	33
1166	FIND keyword	FIND	A keyword in GROUP specification to define selection filters.	identifier|method	93
1167	SEARCH keyword	SEARCH	A keyword in GROUP specification to terminate a FIND block.	identifier|method	75
1168	Self-Guided Langevin Dynamics	SGLD	Enhanced sampling method that accelerates low-frequency motions.	method|algorithm	46
1169	Algorithm Index	isgld	Selects the specific SGLD algorithm to be used.	method|algorithm	16
1170	SGLD Local Averaging Time	tsgavg	Averaging time in picoseconds for guiding force calculation.	measure|unit	13
1171	SGLD Momentum Guiding Factor	sgft	Defines the strength of the momentum-based guiding effect.	measure|parameter	43
1172	SGLD Force Guiding Factor	sgff	Scales the low-frequency energy surface to flatten barriers.	measure|parameter	29
1173	SGLD-GLE Momentum Guiding Factor	sgfg	Momentum guiding factor for the SGLD-GLE method.	measure|parameter	5
1174	SGLD Effective Guiding Temperature	tempsg	Defines the effective temperature of the guiding potential.	measure|state	10
1175	SGLD Start Atom Index	isgsta	The first atom index of the region to apply SGLD.	identifier	4
1176	SGLD End Atom Index	isgend	The last atom index of the region to apply SGLD.	identifier	4
1177	SGLD Atom Mask	sgmask	Amber mask for selecting atoms to apply guiding forces.	identifier|data format	3

1178	SGLD Spatial Average Type	sgtype	Defines the type of spatial averaging for guiding forces.	method|algorithm	3
1179	SGLD Spatial Average Size	sgsize	Cutoff distance for local spatial averaging in Angstroms.	measure|unit	4
1180	Generalized Langevin Equation	SGLD-GLE	SGLD variant that exactly preserves the canonical ensemble.	method|algorithm	7
1181	Accelerated Molecular Dynamics	aMD	Enhanced sampling method adding a bias potential to reduce barriers.	method|algorithm	59
1182	aMD Boost Selection	iamd	Selects which potential energy terms are boosted in aMD.	method|algorithm	8
1183	aMD Dihedral Energy Threshold	EthreshD	Threshold dihedral energy for applying the aMD boost.	measure|parameter	6
1184	aMD Dihedral Alpha Factor	alphaD	Determines the strength of the dihedral energy boost.	measure|parameter	6
1185	aMD Potential Energy Threshold	EthreshP	Threshold total potential energy for applying the aMD boost.	measure|parameter	6
1186	aMD Potential Alpha Factor	alphaP	Determines the strength of the total potential energy boost.	measure|parameter	5
1187	aMD Log File	amd.log	Log file containing aMD boost information for reweighting.	data format|data source	10
1188	aMD Log File Command	-amdlog	Command line option to specify the aMD log file name.	identifier|software	1
1189	Dynamics	LiGaMD	GaMD variant for simulating ligand binding and unbinding.	method|algorithm	17
1190	Dual-Boost Ligand GaMD	LiGaMD_Dual	LiGaMD variant with a second boost on the system.	method|algorithm	5
1191	Dynamics	Pep-GaMD	GaMD variant for sampling peptide-protein interactions.	method|algorithm	12
1192	Dual-Boost Peptide GaMD	Pep-GaMD_Dual	Pep-GaMD variant with a second boost on the system.	method|algorithm	5
1193	Dynamics 3	LiGaMD3	GaMD variant with three distinct boosts for flexible substrates.	method|algorithm	9
1194	Protein-Protein Interaction GaMD	PPI-GaMD	GaMD variant for sampling protein-protein interactions.	method|algorithm	15
1195	Dual-Boost PPI-GaMD	PPI-GaMD_Dual	PPI-GaMD variant with a second boost on the system.	method|algorithm	3
1196	GaMD Boost Selection	igamd	Selects which potential energy terms are boosted in GaMD.	method|algorithm	26
1197	GaMD Threshold Energy Flag	iE	Flag to set the method for calculating threshold energy E.	method|algorithm	21
1198	GaMD First Boost Threshold Flag	iEP	Flag to set threshold energy for the first boost potential.	method|algorithm	6
1199	GaMD Second Boost Threshold Flag	iED	Flag to set threshold energy for the second boost potential.	method|algorithm	6
1200	GaMD Third Boost Threshold Flag	iEB	Flag to set threshold energy for the third boost potential.	method|algorithm	2
1201	GaMD Preparation cMD Steps	ntcmdprep	Number of conventional MD steps for preparation before statistics collection.	measure|process	17
1202	GaMD Initial cMD Steps	ntcmd	Number of conventional MD steps for collecting potential energy statistics.	measure|process	35
1203	GaMD Preparation Biasing Steps	ntebprep	Number of preparation steps after adding the boost potential.	measure|process	17
1204	GaMD Biasing Steps	nteb	Number of biasing MD steps for updating potential statistics.	measure|process	20
1205	GaMD Restart Flag	irest_gamd	Flag to restart a GaMD simulation from a saved state.	state|process	15
1206	GaMD Potential Boost StdDev Limit 1	sigma0P	Upper limit of the standard deviation for the first potential boost.	measure|parameter	7
1207	GaMD Potential Boost StdDev Limit 2	sigma0D	Upper limit of the standard deviation for the second potential boost.	measure|parameter	7
1208	GaMD Potential Boost StdDev Limit 3	sigma0B	Upper limit of the standard deviation for the third potential boost.	measure|parameter	2
1209	GaMD Protein 2 Start Atom	bgpro2atm	Starting atom number of the second protein in PPI-GaMD.	identifier	4
1210	GaMD Protein 2 End Atom	edpro2atm	Ending atom number of the second protein in PPI-GaMD.	identifier	4
1211	Number of Ligands	nlig	Specifies the total number of ligand molecules in the system.	measure	8
1212	Boost Bound Ligand Flag	ibblig	Flag to selectively boost the ligand bound to the protein.	method|algorithm	6
1213	Ligand Distance Protein Atom	atom_p	Serial number of a protein atom for ligand distance calculation.	identifier	4
1214	Ligand Distance Ligand Atom	atom_l	Serial number of a ligand atom for ligand distance calculation.	identifier	4
1215	Ligand Binding Distance Cutoff	dblig	Cutoff distance to determine if a ligand is bound.	measure|unit	3

1216	Targeted MD	Targeted MD	Method to steer a simulation towards a target structure using RMSD restraints.	method|algorithm	18
1217	Targeted MD Flag	itgtmd	Flag to enable Targeted MD or Multiply-Targeted MD.	method|algorithm	3
1218	Target RMSD	tgtrmsd	The target root-mean-square deviation value for the restraint.	measure|parameter	16
1219	Targeted MD Force Constant	tgtmdfrc	Force constant for the targeted MD RMSD restraint.	measure|parameter	5
1220	Targeted MD Fit Mask	tgtfitmask	Atom mask for RMS superposition between current and reference structures.	identifier|data format	7
1221	Targeted MD RMSD Mask	tgtrmsmask	Atom mask for calculating the RMSD for the restraint force.	identifier|data format	9
1222	Multiply-Targeted MD	MTMD	Targeted MD using multiple reference structures simultaneously.	method|algorithm	13
1223	MTMD Namelist	&tgt	Namelist containing parameters for a single MTMD target.	data format	3
1224	MTMD Reference File	refin	Filename of the reference structure for an MTMD target.	data source	5
1225	MTMD Reference File Format	mtmdform	Flag indicating if the MTMD reference file is formatted.	data format	7
1226	MTMD Step Range	mtmdstep1, mtmdstep2	Defines the simulation step range for applying a specific MTMD target.	measure|process	1
1227	MTMD Varying Parameters Flag	mtmdvari	Flag to vary the force constant and target RMSD over time.	method|algorithm	11
1228	MTMD Target RMSD Range	mtmdrmsd, mtmdrmsd2	Initial and final target RMSD values for a varying restraint.	measure|parameter	0
1229	MTMD Force Constant Range	mtmdforce, mtmdforce2	Initial and final force constant values for a varying restraint.	measure|parameter	0
1230	MTMD Update Increment	mtmdninc	Step increment for applying changes in varying MTMD parameters.	measure|process	9
1231	MTMD Multiplicative Scaling Flag	mtmdmult	Flag for multiplicative scaling of the force constant.	method|algorithm	8
1232	MTMD Atom Mask	mtmdmask	Atom mask for both fitting and force calculation for an MTMD target.	identifier|data format	6
1233	Partial Nudged Elastic Band	PNEB	NEB method applied to a user-defined subset of the system.	method|algorithm	5
1234	NEB Flag	ineb	Flag to enable Nudged Elastic Band simulation.	method|algorithm	3
1235	NEB Max Spring Constant	skmax	Maximum spring constant connecting images in NEB.	measure|parameter	4
1236	NEB Min Spring Constant	skmin	Minimum spring constant for scaled-spring NEB calculations.	measure|parameter	5
1237	NEB Tangent Mode	tmode	Selects the tangent definition to prevent path kinks.	method|algorithm	2
1238	NEB Quenched Velocity Verlet Flag	vv	Flag to use the quenched velocity Verlet minimization.	method|algorithm	31
1239	NEB Velocity Scaling Factor	vfac	Scaling factor for the quenched velocity Verlet algorithm.	measure|parameter	2
1240	Collective Variable	CV	A function of atomic coordinates used to describe complex motions.	measure|model	67
1241	Path Collective Variable	pathCV	A collective variable defined along an optimized reaction path.	measure|model	11
1242	ASM Namelist	&asm	Namelist containing options for the Adaptive String Method.	data format	1
1243	ASM Guess Path File	guess_file	Path to the file providing the initial guess for the path.	data source	1
1244	ASM PMF-only Flag	only_PMF	Flag to start an ASM calculation directly from the PMF stage.	process|state	3
1245	ASM Replica Exchange Period	REX_period	Period in timesteps for attempting replica exchange between nodes.	measure|process	1
1246	ASM Preparation Steps	preparation_steps	Duration of the preparation stage for gradually increasing force constants.	measure|process	3
1247	Grote-Hynes Theory Analysis Flag	grote_hynes	Flag to enable analysis based on Grote-Hynes theory.	method|analysis	2
1248	XMIN Minimization	XMIN	A suite of fast local energy minimization techniques.	method|algorithm	26
1249	ARPACK	ARPACK	A software library for solving large scale eigenvalue problems.	software	15
1250	Polak-Ribiere Conjugate Gradient	PRCG	A specific nonlinear conjugate gradient minimization algorithm.	algorithm|method	3
1251	Limited-memory BFGS	LBFGS	A quasi-Newton minimization algorithm for large problems.	algorithm|method	13
1252	Truncated Newton Conjugate Gradient	TNCG	A minimization method using a truncated Newton approach.	algorithm|method	7
1253	LMOD/XMIN Namelist	&lmod	Namelist containing options for LMOD and XMIN methods.	data format	3

1254	ARPACK Arnoldi Dimension	arnoldi_dimension	Dimension of the Arnoldi factorization used by ARPACK.	measure|parameter	6
1255	LMOD Conformational Library	conflib_filename	Filename for the library of low-energy conformations found by LMOD.	data format|data source	2
1256	LMOD Monte Carlo Method	monte_carlo_method	Selects the Monte Carlo method for exploring conformations.	method|algorithm	1
1257	DL-Find	DL-Find	An open-source suite of geometry optimization algorithms.	software|method	9
1258	libdlfind	libdlfind	The specific library version of DL-Find linked to Sander.	software	2
1259	DL-Find Namelist	&dlfind	Namelist containing options for the DL-Find optimizer.	data format	3
1260	DL-Find Active Atoms	active	Amber mask specifying which atoms are allowed to move during optimization.	identifier|data format	103
1261	DL-Find Coordinate Representation	crdrep	Specifies the coordinate system for geometry optimization (e.g., HDLC).	method|model	4
1262	DL-Find Optimization Algorithm	optalg	Selects the optimization algorithm (e.g., LBFGS, PRFO).	algorithm|method	9
1263	DL-Find Trust Radius	trustrad	Specifies the approach for adjusting the trust radius during optimization.	method|algorithm	2
1264	DL-Find Initial Hessian	hessini	Specifies how the initial Hessian matrix is approximated.	method|algorithm	3
1265	DL-Find Hessian Update	hessupd	Specifies the method for updating the approximate Hessian.	method|algorithm	4
1266	Dimer Method Flag	dimer	Logical flag to enable the dimer method for TS search.	method|algorithm	9
1267	NEB Number of Images	neb_nimage	The number of images to optimize along the path.	measure|parameter	2
1268	NEB Climbing Image Test	neb_climb_test	Threshold for spawning a climbing image to find the saddle point.	measure|parameter	3
1269	NEB Freezing Image Test	neb_freeze_test	Threshold for freezing NEB images during optimization.	measure|parameter	2
1270	NEB Spring Constant	nebk	The spring force constant connecting adjacent NEB images.	measure|parameter	2
1271	NEB Cartesian Optimization	neb_cart	Flag to perform NEB optimization in Cartesian coordinates.	method|algorithm	2
1272	Free Energy	Free Energy	A thermodynamic potential that measures the useful work obtainable from a system.	measure|state	312
1273	TI Free Energy Flag	icfe	Flag to enable thermodynamic integration free energy calculations.	method|process	20
1274	TI Lambda Value	clambda	The value of the coupling parameter lambda for a TI simulation.	measure|parameter	19
1275	TI Lambda Exponent	klambda	The exponent used in the non-linear mixing rule for TI.	measure|parameter	10
1276	TI SHAKE Handling	tishake	Flag that determines how SHAKE constraints are handled in TI.	method|algorithm	11
1277	TI Mask for V1	timask2	Specifies atoms unique to the final state V1 in pmemd TI.	identifier|data format	15
1278	Gaussian Quadrature	Gaussian Quadrature	A numerical method for approximating the definite integral of a function.	algorithm|method	1
1279	Linear Mixing	Linear Mixing	A potential energy function that is a linear interpolation between two states.	model|method	3
1280	Softcore Potential	Softcore Potential	A modified potential function to avoid singularities when atoms appear/disappear.	model|method	8
1281	Softcore Potential Flag	ifsc	Flag to enable the use of softcore potentials in TI.	method|model	22
1282	Softcore Alpha Parameter	scalpha	The alpha parameter in the softcore van der Waals potential.	measure|parameter	6
1283	Log dV/dL Flag	logdvdl	Flag to write a summary of all dV/dlambda values for postprocessing.	process|software	2
1284	Charge Mask	crgmask	Specifies atoms that will have their partial charges set to zero.	identifier|data format	6
1285	Softcore Mask (Sander)	scmask	Specifies the unique softcore atoms for a process in sander.	identifier|data format	11
1286	Softcore Mask for V1 (PMEMD)	scmask2	Specifies the unique softcore atoms for state V1 in pmemd.	identifier|data format	19
1287	Softcore Beta Parameter	scbeta	The beta parameter in the softcore electrostatic potential.	measure|parameter	10
1288	Smoothstep Function	Smoothstep	A family of sigmoid-like interpolation functions with zero derivatives at endpoints.	model|algorithm	20
1289	Lambda-Scheduling	lambda-scheduling	A technique using smoothstep functions to control the alchemical transformation path.	method|algorithm	9
1290	Lambda-Scheduling Flag	gti_lam_sch	Flag to enable lambda-scheduling in pmemd.cuda TI simulations.	method|algorithm	8
1291	Electrostatic Softcore Flag	gti_ele_sc	Flag to utilize smoothstep functions for electrostatic softcore potentials.	method|model	2

1292	VDW Softcore Flag	gti_vdw_sc	Flag to utilize smoothstep functions for van der Waals softcore potentials.	method|model	2
1293	Scale Beta Flag	gti_scale_beta	Flag to enable a new form of softcore potential with unit-less beta.	method|model	4
1294	VDW Softcore Exponent	gti_vdw_exp	The exponent 'n' in the modified softcore VDW potential.	measure|parameter	2
1295	Electrostatic Softcore Exponent	gti_ele_exp	The exponent 'm' in the modified softcore electrostatic potential.	measure|parameter	2
1296	Softcore Tail Smoothing Flag	gti_cut_sc	Flag to enable tail smoothing to the softcore potential.	method|model	4
1297	Softcore Interaction Control	gti_add_sc	Flag to control how interactions involving softcore regions are treated.	method|model	13
1298	Softcore Bonded Term Control	gti_bat_sc	Flag to control how bonded terms involving softcore regions are treated.	method|model	7
1299	Softcore Bond Mask 1	sc_bond_mask1	Mask to select non-scaled bond terms for softcore region 1.	identifier|data format	8
1300	Softcore Bond Mask 2	sc_bond_mask2	Mask to select non-scaled bond terms for softcore region 2.	identifier|data format	1
1301	Softcore Angle Mask 1	sc_angle_mask1	Mask to select non-scaled angle terms for softcore region 1.	identifier|data format	2
1302	Softcore Angle Mask 2	sc_angle_mask2	Mask to select non-scaled angle terms for softcore region 2.	identifier|data format	1
1303	Softcore Torsion Mask 1	sc_torsion_mask1	Mask to select non-scaled torsion terms for softcore region 1.	identifier|data format	2
1304	Softcore Torsion Mask 2	sc_torsion_mask2	Mask to select non-scaled torsion terms for softcore region 2.	identifier|data format	1
1305	Mass Synchronization Flag	gti_syn_mass	Flag to control mass synchronization of common atoms in TI.	method|process	3
1306	VDW Zeroing Mask	ti_vdw_mask	Mask to select atoms whose VDW interactions will be zeroed out.	identifier|data format	2
1307	Detailed TI Output Flag	gti_output	Flag to output term-by-term detailed TI results.	process|software	2
1308	CPU-compatible TI Output Flag	gti_cpu_output	Flag to ensure TI output matches the CPU version's format.	process|software	7
1309	Internal Softcore Cutoff Flag	gti_cut	Flag to control whether internal softcore non-bonded terms are cut.	method|process	3
1310	Softcore Charge Neutralization Flag	gti_chg_keep	Flag to control whether charges of softcore atoms are neutralized.	method|process	2
1311	FEP/MBAR Flag	ifmbar	Flag to generate output for FEP or MBAR postprocessing.	method|process	5
1312	MBAR States	mbar_states	The number of lambda windows considered in an MBAR calculation.	measure|parameter	2
1313	MBAR Lambda Values	mbar_lambda	A list of the lambda values for all simulated states.	measure|parameter	2
1314	LIE Calculation Flag	ilrt	Flag to turn on the computation of Linear Interaction Energy contributions.	method|process	1
1315	LIE Interval	lrt_interval	The frequency in MD steps to compute LIE contributions.	measure|process	3
1316	LIE Solute Mask	lrtmask	Atom mask defining the 'solute' for LIE calculations.	identifier|data format	2
1317	Expanded Ensemble	Expanded Ensemble	A statistical ensemble that includes thermodynamic state parameters as variables.	model|state	8
1318	Detailed Balance	Detailed Balance	A condition ensuring a reversible Markov chain in Monte Carlo methods.	state|concept	4
1319	Number of Exchanges	numexchg	The total number of replica exchange attempts to be performed.	measure|process	12
1320	Asynchronous H-REMD Flag	gremd_acyc	Flag to disable exchanges between the first and last replicas in H-REMD.	method|algorithm	3
1321	REMD Type Flag	-rem	Command-line flag to define the type of 1D REMD simulation.	identifier|software	28
1322	Random Partner Exchange Flag	-remrandompartner	Flag to enable random partner selection for replica exchanges.	method|algorithm	1
1323	genremdinputs.py	genremdinputs.py	A Python tool to generate input files for REMD simulations.	software	21
1324	H-REMD dimension 1	HAMILTONIAN1	Identifier for the first Hamiltonian dimension in a multi-dimensional REMD.	identifier|method	3
1325	H-REMD dimension 2	HAMILTONIAN2	Identifier for the second Hamiltonian dimension in a multi-dimensional REMD.	identifier|method	3
1326	REMD Exchange Probability	P_i,j	The probability of a successful exchange between replicas i and j.	measure|state	0
1327	REMD NetCDF Restart	ntxo=2	Flag to write restart files in the NetCDF binary format.	data format|process	3
1328	REMD NetCDF Trajectory	ioutfm=1	Flag to write trajectory files in the NetCDF binary format.	data format|process	4
1329	Hybrid Solvent REMD	Hybrid-REMD	REMD method using a hybrid explicit/implicit solvent model for exchange calculations.	method|algorithm	2

1330	Number of Waters to Keep	numwatkeep	Number of explicit water molecules retained in the hybrid solvent model.	measure|parameter	5
1331	Hybrid GB Model	hybridgb	Specifies the Generalized Born model used in the hybrid solvent calculation.	model|method	4
1332	Reservoir REMD	Reservoir REMD	ensemble.	method|algorithm	6
1333	Reservoir File Prefix	-reservoir	Command-line flag specifying the file name prefix for reservoir structures.	identifier|data source	1
1334	Reservoir Energies File	-saveene	Command-line flag specifying the file with energies of reservoir structures.	identifier|data source	1
1335	Reservoir Cluster Info File	-clusterinfo	File specifying dihedral definitions for non-Boltzmann reservoir weighting.	data format|data source	1
1336	Perturbation	REFEP	A method combining H-REMD and FEP to calculate free energy differences.	method|process	5
1337	Replica Exchange Umbrella Sampling	REUS	A method combining H-REMD and umbrella sampling for enhanced sampling.	method|algorithm	1
1338	of Freedom	REAF	A REST2-like enhanced sampling method using a tau parameter.	method|algorithm	32
1339	REAF Flag	ifreaf	Flag to enable REAF enhanced sampling.	method|algorithm	3
1340	REAF Tau Parameter	reaf_tau	The tau parameter that controls the scaling of interactions in REAF.	measure|parameter	7
1341	REAF Effective Temperature	reaf_temp	The effective temperature corresponding to a given tau value in REAF.	measure|state	3
1342	REAF Mask 1	reaf_mask1	Amber mask defining the REAF region for the lambda=0 state.	identifier|data format	4
1343	REAF Mask 2	reaf_mask2	Amber mask defining the REAF region for the lambda=1 state.	identifier|data format	3
1344	Multidimensional REMD Namelist	&multirem	Namelist defining a dimension in a multi-dimensional REMD simulation.	data format	5
1345	Multidimensional REMD Exchange Type	exch_type	Defines the type of exchange for a given dimension (e.g., TEMPERATURE).	identifier|method	5
1346	Multidimensional REMD Group Definition	group	Array defining the replica groupings for a specific dimension.	identifier|data format	274
1347	fixremdcouts.py	fixremdcouts.py	A Python tool to reconstruct cpout/ceout files from any REMD simulation.	software	5
1348	Potential of Mean Force	Potential of Mean Force	The free energy profile along a given reaction coordinate.	measure|state	2
1349	Non-equilibrium Free Energy Flag	infe	Flag to enable ABMD and related non-equilibrium free energy methods.	method|process	17
1350	Collective Variable Atom Indices	cv_i	List of atom indices defining a collective variable.	identifier|data format	46
1351	Collective Variable Real Parameters	cv_r	List of real number parameters for a collective variable.	measure|parameter	16
1352	Distance CV	DISTANCE	Reaction coordinate defined as the distance between two atoms.	measure|model	266
1353	Center of Mass Distance CV	COM_DISTANCE	Reaction coordinate defined as the distance between two centers of mass.	measure|model	3
1354	Difference of COM Distances CV	DF_COM_DISTANCE	Reaction coordinate defined as the difference of two COM distances.	measure|model	3
1355	Linear Combination of Distances CV	LCOD	Reaction coordinate defined as a linear combination of distances.	measure|model	2
1356	Center of Mass Angle CV	COM_ANGLE	Reaction coordinate defined as the angle formed by three centers of mass.	measure|model	1
1357	Torsion CV	TORSION	Reaction coordinate defined as the dihedral angle formed by four atoms.	measure|model	146
1358	Center of Mass Torsion CV	COM_TORSION	Reaction coordinate defined as the dihedral angle formed by four centers of mass.	measure|model	1
1359	Sum of Cosines of Dihedrals CV	COS_OF_DIHEDRAL	Reaction coordinate defined as the sum of cosines of dihedral angles.	measure|model	1
1360	Sum of Sines of Dihedrals CV	SIN_OF_DIHEDRAL	Reaction coordinate defined as the sum of sines of dihedral angles.	measure|model	2
1361	Paired Dihedral CV	PAIR_DIHEDRAL	Reaction coordinate based on the sum of cosines of adjacent dihedral pairs.	measure|model	3
1362	Pattern Dihedral CV	PATTERN_DIHEDRAL	A pattern-recognizing function based on a list of dihedral angles.	measure|model	3
1363	Radius of Gyration CV	R_OF_GYRATION	Reaction coordinate defined as the radius of gyration of a group of atoms.	measure|model	1
1364	Multi-RMSD CV	MULTI_RMSD	Reaction coordinate defined as the RMS of RMSDs of several atom groups.	measure|model	4
1365	Number of Bonds CV	N_OF_BONDS	A switching function that counts the number of bonds formed between atom pairs.	measure|model	2
1366	Handedness CV	HANDEDNESS	A reaction coordinate that measures the chirality or handedness of a structure.	measure|model	1
1367	Quaternion	QUATERNIONS	A four-component vector for describing orientational changes of atomistic domains	model|measure	20

1368	Orientation Quaternion	orientation quaternion	A unit quaternion parametrizing the optimal rotation between coordinate sets	model|measure	3
1369	ORIENTATION_ANGLE	ORIENTATION_ANGLE	The angle of rotation between current and reference positions	measure	3
1370	ORIENTATION_PROJ	ORIENTATION_PROJ	The cosine of the angle of rotation between positions	measure	4
1371	TILT	TILT	Cosine of the rotation orthogonal to a given axis	measure	9
1372	SPINANGLE	SPINANGLE	Angle of rotation around a given unit axis	measure	8
1373	QUATERNION0	QUATERNION0	The scalar component (q0) of the orientation quaternion	measure|identifier	10
1374	QUATERNION1	QUATERNION1	The first vector component (q1) of the orientation quaternion	measure|identifier	4
1375	QUATERNION2	QUATERNION2	The second vector component (q2) of the orientation quaternion	measure|identifier	4
1376	QUATERNION3	QUATERNION3	The third vector component (q3) of the orientation quaternion	measure|identifier	9
1377	q_index	q_index	An attribute to link and normalize quaternion CVs together	identifier	8
1378	&smd namelist	&smd	Namelist in the MDIN file to activate steered MD	data format	8
1379	Catmull-Rom spline	Catmull-Rom spline	A spline used for defining the steering path or harmonic constant	model|algorithm	2
1380	path_mode	path_mode	Defines how steering paths are constructed (SPLINE or LINES)	identifier	4
1381	harm	harm	Specifies the harmonic constant for the steering potential	measure	7
1382	Umbrella Sampling	Umbrella sampling	A method using biasing potentials to enhance sampling along a coordinate	method|process	27
1383	&pmd namelist	&pmd	Namelist in the MDIN file to activate umbrella sampling	data format	8
1384	anchor_position	anchor_position	Determines the boundaries of the umbrella harmonic potential	measure	9
1385	anchor_strength	anchor_strength	Sets the harmonic constant for the umbrella potential	measure	11
1386	&abmd namelist	&abmd	Namelist in the MDIN file to activate ABMD	data format	15
1387	&bbmd namelist	&bbmd	Namelist for replica-exchange ABMD with different reaction coordinates	data format	13
1388	FLOODING mode	FLOODING	ABMD execution mode where adaptive biasing is enabled	state|method	15
1389	timescale	timescale	The flooding timescale (τF) in picoseconds for ABMD	measure|unit	9
1390	Multiple-walker selection algorithm	algorithm	Improves ABMD simulation by resampling between different walkers	algorithm|method	2
1391	wt_temperature	wt_temperature	Sets the pseudo-temperature for well-tempered ABMD	measure	3
1392	&stsm namelist	&stsm	Namelist in the MDIN file to invoke the STSM	data format	7
1393	image	image	A node defining a point on the string in STSM	identifier|model	63
1394	nfe-umbrella-slice	nfe-umbrella-slice	A utility to process and analyze biasing potential files from ABMD	software	10
1395	Jarzynski Relationship	Jarzynski relationship	Relates non-equilibrium work to equilibrium free energy differences	model|method	2
1396	.RST file	.RST	A file specifying restraint conditions for SMD or NMR	data format	1
1397	EMIL	EMIL	A method to calculate absolute free energy via thermodynamic integration	method|algorithm	52
1398	Einstein Molecule	Einstein Molecule	A reference system with an analytically known free energy	model	1
1399	emil_do_calc	emil_do_calc	A flag in the input file to activate EMIL calculation	identifier	3
1400	emilParameters.in	emilParameters.in	An EMIL-specific input file for control data	data format|data source	7
1401	emil_sc	emil_sc	Option for mutual softcoring of interatomic forces in EMIL	identifier|method	9
1402	softcoring	softcoring	A technique to avoid singularities in potential energy calculations	method|algorithm	3
1403	solidRes	solidRes	List of residues with atoms assigned to specific harmonic wells	identifier	5
1404	liquidRes	liquidRes	List of residues part of a fluid with adjustable well assignments	identifier	9
1405	ijarzynski	ijarzynski	An input parameter to enable features for Jarzynski's equation calculations	identifier	7

1406	icnstph	icnstph	Input flag to turn on constant pH simulations	identifier	4
1407	solvph	solvph	Input parameter to set the solvent pH value	measure	11
1408	ntcnstph	ntcnstph	Number of MD steps between protonation state change attempts	measure	6
1409	ntrelax	ntrelax	Number of solvent relaxation steps after a protonation state change	measure	4
1410	cprestrt file	cprestrt	A restart file for constant pH simulations	data format	8
1411	cpinutil.py	cpinutil.py	A python script to generate the cpin file	software	21
1412	finddgref.py	finddgref.py	A tool to automatically compute reference energies for CpHMD	software|method	26
1413	reference energy	reference energy	Pre-computed energy difference for a protonation state change	measure	15
1414	AS4	AS4	A special residue name for titratable aspartic acid	chemical entity	30
1415	GL4	GL4	A special residue name for titratable glutamic acid	chemical entity	24
1416	leaprc.constph	leaprc.constph	A LEaP command file for preparing constant pH systems	data source	2
1417	Henderson-Hasselbalch equation	equation	Relates pH, pKa, and the ratio of protonated/deprotonated species	model	1
1418	Hill equation	Hill equation	Describes ligand binding to macromolecules, used for pKa fitting	model	1
1419	calcpka	calcpka	A program for calculating pKa values from simulation data	software	16
1420	Conditional Probability	Conditional Probabilities	The probability of an event given another event has occurred	measure	24
1421	Dynamics	molecular dynamics	A method to simulate systems at a constant redox potential	method|process	1
1422	CEMD	CEMD	Acronym for Constant Redox Potential Molecular Dynamics	method|process	1
1423	cein file	cein file	An input file describing redox-active titrating residues and states	data format|data source	22
1424	HEH	HEH	A redox-active residue representing a bis-histidine heme group	chemical entity	7
1425	leaprc.conste	leaprc.conste	A LEaP command file for preparing constant redox potential systems	data source	2
1426	ceinutil.py	ceinutil.py	A python tool to generate the cein input file	software	10
1427	cpeinutil.py	cpeinutil.py	A tool for residues that are both pH- and redox-active	software	2
1428	cpein file	cpein file	Input file for simultaneously pH- and redox-active residues	data format|data source	2
1429	icnste	icnste	An input flag to enable constant redox potential simulations	identifier	3
1430	solve	solve	An input parameter to set the solvent redox potential in Volts	measure|identifier|unit	16
1431	ntcnste	ntcnste	The number of MD steps between redox state change attempts	measure|identifier	3
1432	ntrelaxe	ntrelaxe	The number of solvent relaxation steps after a redox state change	measure|identifier	3
1433	ceout file	ceout file	An output file logging the history of sampled redox states	data format	4
1434	Nernst equation	Nernst equation	Relates reduction potential to standard potential and concentrations	model	1
1435	Continuous constant pH MD	MD	An alternative CpHMD method using lambda-dynamics for continuous titration	method|algorithm	5
1436	lambda-dynamics	lambda-dynamics	A free energy calculation method using a dynamic coupling parameter	method|algorithm	0
1437	iphmd	iphmd	An input flag to select the continuous CpHMD mode	identifier	7
1438	GBNeck2	GBNeck2	A specific Generalized Born implicit solvent model	model	8
1439	phmd.lib	phmd.lib	A library file with residue definitions for continuous CpHMD	data source	1
1440	frcmod.phmd	frcmod.phmd	A force field modification file for continuous CpHMD	data source	1
1441	AS2	AS2	A residue definition for ASP with two dummy hydrogens	chemical entity	6
1442	GL2	GL2	A residue definition for GLU with two dummy hydrogens	chemical entity	6
1443	PME-CpHMD	PME-CpHMD	All-atom continuous CpHMD using Particle Mesh Ewald for electrostatics	method|algorithm	4

1444	&phmdin namelist	&phmdin	A namelist for continuous CpHMD input parameters	data format	3
1445	&phmdparm namelist	&phmdparm	A namelist for continuous CpHMD model compound/peptide parameters	data format	3
1446	NMR refinement	NMR refinement	A process of using NMR data to refine biomolecular structures	process|method	10
1447	J-coupling	J-coupling	A measure of through-bond interactions used for dihedral restraints	measure	15
1448	Residual Dipolar Couplings	residual dipolar couplings	A measure of bond vector orientation in a magnetic field	measure	3
1449	&rst namelist	&rst	A namelist for defining individual restraints in the DISANG file	data format	22
1450	iat	iat	An array of atom indices that define a restraint	identifier	72
1451	Generalized distance coordinate restraint	coordinate restraint	A restraint defined as a linear combination of multiple distances	model|measure	2
1452	Karplus relationship	Karplus relationship	An equation that relates J-coupling values to dihedral angles	model	2
1453	rjcoef	rjcoef	Coefficients (A, B, C) for the Karplus relationship	measure|identifier	16
1454	NOESY volume restraints	NOESY volume restraints	Restraints based on integrated NOESY cross-peak intensities	measure|method	3
1455	&noeexp namelist	&noeexp	A namelist for defining NOESY volume restraint experiments	data format	7
1456	Chemical shift restraints	Chemical shift restraints	Restraints based on differences between observed and calculated chemical shifts	measure|method	4
1457	&shf namelist	&shf	A namelist for defining chemical shift restraints	data format	2
1458	Pseudocontact shift restraints	restraints	Restraints based on chemical shifts induced by paramagnetic centers	measure|method	1
1459	&pcshift namelist	&pcshift	A namelist for defining pseudocontact shift restraints	data format	1
1460	Magnetic susceptibility tensor	tensor	Describes the magnetic properties and anisotropy of a paramagnetic center	model|measure	4
1461	Direct dipolar coupling restraints	restraints	Restraints based on direct dipolar couplings in partially aligned media	measure|method	3
1462	&align namelist	&align	A namelist for defining dipolar coupling restraints and alignment tensors	data format	4
1463	Alignment tensor	alignment tensor	Describes the average orientation of a molecule in a sample	model|measure	20
1464	Residual CSA restraints	Residual CSA restraints	Restraints based on chemical shift anisotropy in partially aligned media	measure|method	0
1465	&csa namelist	&csa	A namelist for defining residual CSA restraints	data format	1
1466	cyanarest_to_amberRST	cyanarest_to_amberRST	A program to convert Cyana restraints to Amber format	software	1
1467	addles	addles	A program to prepare topology and coordinate files for LES simulations	software	24
1468	tordef.lib	tordef.lib	A default library file defining standard torsion angles for makeANG_RST	data source	1
1469	makeDIP_RST	makeDIP_RST	A program to prepare residual dipolar coupling restraint files	software	7
1470	NMR Exchange Format	NEF	A common, standard format for encoding and exchanging NMR restraints	data format	8
1471	fantasian	fantasian	A program to evaluate magnetic anisotropy tensor parameters from pseudocontact shifts	software	5
1472	sander.LES	sander.LES	A version of the sander program that supports LES simulations	software	2
1473	&emap namelist	&emap	A namelist in the input file containing parameters for an EMAP restraint	data format	7
1474	mapfile	mapfile	The filename of a restraint map or structure for EMAP restraints	data source|identifier	9
1475	atmask	atmask	An atom mask string for selecting atoms to be restrained	identifier	6
1476	fcons	fcons	The restraining force constant for an EMAP restraint	measure	6
1477	FRETrest	FRETrest	A set of scripts for generating FRET-based restraints for MD simulations	software|method	10
1478	placeAV.py	placeAV.py	A script that adds pseudo atoms representing fluorescent dyes to a topology file	software	2
1479	FRETrest.py	FRETrest.py	A script that applies FRET restraints between pseudo atoms	software	3
1480	X-ray refinement	X-ray refinement	The process of refining a molecular structure using X-ray diffraction data	method|process	1
1481	Structure factors	Structure factors	The Fourier transform of the electron density, used in crystallographic refinement	measure|model	3

1482	Miller indices	h, k, l	A set of three integers that identify a specific reflection in crystallography	identifier	2
1483	&xray namelist	&xray	A namelist in the mdin file containing parameters for X-ray refinement	data format	3
1484	reflection_infile	reflection_infile	An input file containing experimental structure factors and R-free flags	data source	3
1485	bulk_solvent_model	bulk_solvent_model	A model to account for the contribution of disordered solvent to diffraction	model	4
1486	Maximum Likelihood target function	target = 'ml'	A statistical target function used for X-ray refinement	model|method	1
1487	&amoeba namelist	&amoeba	A namelist in the input file containing parameters for an AMOEBA simulation	data format	8
1488	&gem namelist	&gem	A namelist in the input file containing parameters for a GEM* simulation	data format	5
1489	Beeman integrator	beeman_integrator	A dynamics integrator algorithm, an alternative to velocity Verlet	algorithm	4
1490	iextpot	iextpot	An input flag to enable an external potential, such as KMMD	identifier	6
1491	NAB	NAB	A scripting language (Nucleic Acid Builder) for manipulating macromolecular structures	software	27
1492	sff	sff	A "simple force field" library within NAB for molecular mechanics calculations	software|model	7
1493	ambpdb	ambpdb	A utility to convert Amber coordinate/restart files to the PDB format	software	21
1494	MM/PB(GB)SA	MM/PB(GB)SA	A post-processing method to estimate binding free energies from snapshots	method|algorithm	6
1495	iAPBS	iAPBS	An interface to the Adaptive Poisson Boltzmann Solver (APBS) program	software|interface	8
1496	ante-MMPBSA.py	ante-MMPBSA.py	A python utility to create compatible topology files for MMPBSA.py	software	6
1497	single trajectory protocol	single trajectory protocol	An MM/PB(GB)SA approach using one trajectory for all species	method	1
1498	multiple trajectory protocol	multiple trajectory protocol	An MM/PB(GB)SA approach using separate trajectories for each species	method	2
1499	&general namelist	&general	A namelist in the MMPBSA.py input file for general parameters	data format	13
1500	&gb namelist	&gb	A namelist in the MMPBSA.py input file for Generalized Born parameters	data format	12
1501	&alanine_scanning namelist	&alanine_scanning	A namelist in the MMPBSA.py input file for alanine scanning parameters	data format	4
1502	&nmode namelist	&nmode	A namelist in the MMPBSA.py input file for normal mode analysis parameters	data format	4
1503	&decomp namelist	&decomp	A namelist in the MMPBSA.py input file for energy decomposition parameters	data format	4
1504	endframe	endframe	The final frame to extract from a trajectory for analysis	identifier	9
1505	interval	interval	The offset for choosing frames from a trajectory	identifier	59
1506	keep_files	keep_files	A variable specifying which temporary files to keep after a run	identifier	8
1507	receptor_mask	receptor_mask	An Amber mask specifying the receptor residues in the complex	identifier	6
1508	startframe	startframe	The first frame to extract from a trajectory for analysis	identifier	10
1509	strip_mask	strip_mask	An Amber mask specifying atoms to be stripped from a trajectory	identifier	9
1510	use_sander	use_sander	A flag to force the use of the sander program for calculations	identifier	4
1511	qm_residues	qm_residues	A list of residues to be treated with quantum mechanics	identifier	3
1512	qmcharge_com	qmcharge_com	The total charge of the quantum mechanical region of the complex	measure	1
1513	qmcharge_lig	qmcharge_lig	The total charge of the quantum mechanical region of the ligand	measure	1
1514	qmcharge_rec	qmcharge_rec	The total charge of the quantum mechanical region of the receptor	measure	1
1515	surfoff	surfoff	An offset to correct the non-polar contribution to solvation free energy	measure	3
1516	probe	probe	The radius of the probe molecule for molecular surface calculation	measure	28
1517	cavity_surften	cavity_surften	The surface tension value for PB non-polar energy calculation	measure	5
1518	exdi	exdi	The external dielectric constant for PB calculations	measure	7
1519	indi	indi	The internal dielectric constant for PB calculations	measure	8

1520	linit	linit	The maximum number of iterations for the linear PB equation	identifier	6
1521	prbrad	prbrad	The solvent probe radius for PB calculations	measure	6
1522	sander_apbs	sander_apbs	A flag to use the APBS program for PB calculations via an interface	identifier	3
1523	memopt	memopt	A flag to turn on membrane protein support in PB calculations	identifier	4
1524	emem	emem	The dielectric constant of the membrane	measure	3
1525	mutant_only	mutant_only	A flag to perform calculations only for the mutant in alanine scanning	identifier	3
1526	nminterval	nminterval	The interval for selecting frames for normal mode calculations	identifier	3
1527	nmendframe	nmendframe	The final frame for normal mode calculations	identifier	3
1528	nmode_igb	nmode_igb	The Generalized Born model to use for normal mode calculations	identifier	3
1529	nmode_istrng	nmode_istrng	The ionic strength for normal mode calculations	measure|unit	2
1530	nmstartframe	nmstartframe	The starting frame for normal mode calculations	identifier	3
1531	print_res	print_res	A selection of residues for which to print decomposition results	identifier	5
1532	solvcut	solvcut	The cutoff for solute-solvent interactions in 3D-RISM	measure	8
1533	thermo	thermo	The thermodynamic equation to use for calculating RISM solvation properties	identifier	4
1534	MMPBSA.py API	MMPBSA.py API	A Python Application Programming Interface for accessing MMPBSA.py data	software|interface	1
1535	load_mmpbsa_info	load_mmpbsa_info	A function in the MMPBSA.py API to load and parse calculation data	software	6
1536	mmpbsa_data	mmpbsa_data	A data structure (dictionary) in the API that holds parsed MMPBSA.py results	data format	14
1537	WAMM	WAMM	A FEW module for automated MM-PBSA & MM-GBSA calculations	software|process	8
1538	LIEW	LIEW	A FEW module for Linear Interaction Energy workflow	software|process	4
1539	TIW	TIW	A FEW module for Thermodynamic Integration workflow	software|process	5
1540	1-trajectory protocol	1-trajectory protocol	An MM-PB(GB)SA approach using a single trajectory for all species	method	0
1541	3-trajectory protocol	3-trajectory protocol	An MM-PB(GB)SA approach using separate trajectories for complex, receptor, and ligand	method	1
1542	mbondi radii	mbondi	A set of atomic radii for implicit solvent calculations	data source|model	15
1543	Hawkins-Cramer-Truhlar radii	GB^HTC	Radii set used for specific Generalized Born calculations	data source|model	0
1544	Linear Combination of Pairwise Overlaps	LCPO	Method to calculate solvent accessible surface area	algorithm|method	11
1545	Bondi radii	bondi	A standard set of van der Waals radii for atoms	data source|model	12
1546	Tan&Luo radii	Tan&Luo	Atomic radii set optimized for Poisson-Boltzmann calculations	data source|model	4
1547	Hybrid Solvent MM-PBSA	Hybrid PBSA	A hybrid MM-PBSA calculation method	method|model	2
1548	Molecular Surface Area	MSA	The surface area of a molecule, often solvent-excluded	measure	5
1549	Parse radii	Parse	A set of atomic radii for Poisson-Boltzmann calculations	data source|model	17
1550	ICOSA	ICOSA	A recursive approximation method for calculating SASA from an icosahedron	algorithm|method	2
1551	Gradient	Choleski Conjugate	A numerical solver for the Poisson-Boltzmann equation	algorithm	1
1552	Ligand Structure Path	lig_struct_path	Path to the directory containing ligand structure files	identifier	5
1553	Output Path	output_path	Path to the main output directory for calculations	identifier	19
1554	Water in Receptor	water_in_rec	Flag indicating if crystal waters are present in the receptor	identifier|state	3
1555	MM-PBSA Calculation Setup	mmpbsa_calc	Flag to request setup of MM-PBSA/MM-GBSA calculation files	process	2
1556	Trajectory Approach	1_or_3_traj	Specifies using a single or three separate trajectories	method|identifier	15
1557	Additional Library	additional_library	Path to a library file for non-standard residues	data source|identifier	9

1558	Additional Frcmod	additional_frcmod	Path to a force field modification file with extra parameters	data source|identifier	6
1559	mm_pbsa.pl	mmpbsa_pl	The main Perl script for running MM-PBSA/GBSA calculations	software	11
1560	Snapshot Extraction	extract_snapshots	Flag to request extraction of coordinate frames from a trajectory	process	6
1561	First Snapshot	first_snapshot	Index of the first trajectory frame to be extracted	identifier	4
1562	Last Snapshot	last_snapshot	Index of the last trajectory frame to be extracted	identifier	4
1563	Offset Snapshots	offset_snapshots	Frequency or step size for extracting trajectory frames	identifier	2
1564	Trajectory Files	trajectory_files	Specifies which trajectory files to use for snapshot extraction	data source|identifier	24
1565	Image Trajectories	image_trajectories	Flag to center and re-orient molecules in trajectory snapshots	process	2
1566	Use Imaged Trajectories	use_imaged_trajectories	Flag to reuse previously imaged trajectories for subsequent calculations	identifier|state	3
1567	Image Mass Origin	image_mass_origin	Flag to image the system relative to its mass origin	process|identifier	1
1568	Number of Receptor Residues	no_of_rec_residues	The total count of amino acid residues in the receptor	measure|identifier	3
1569	Total Number of Intervals	total_no_of_intervals	Total number of trajectory segments to be analyzed	identifier	2
1570	First PB Snapshot	first_PB_snapshot	The starting snapshot for the MM-PBSA/GBSA analysis	identifier	2
1571	Last PB Snapshot	last_PB_snapshot	The ending snapshot for the MM-PBSA/GBSA analysis	identifier	2
1572	Offset PB Snapshots	offset_PB_snapshots	The frequency of snapshots to use in the MM-PBSA/GBSA analysis	identifier	2
1573	Parallel MM-PBSA Calculation	parallel_mmpbsa_calc	Number of processors to use for a parallel calculation	identifier	1
1574	Implicit Membrane	implicit_membrane	Flag to include a low-dielectric slab representing a membrane	model|identifier	25
1575	APBS Executable	apbs_executable	Full path to the APBS software executable file	identifier|software	2
1576	Bottom Membrane Boundary	dary	The lower z-coordinate boundary of the implicit membrane slab	measure	2
1577	Membrane Thickness	membrane_thickness	The total thickness of the implicit membrane slab in Angstroms	measure	7
1578	Membrane Dielectric Constant	membrane_dielc	The dielectric constant of the main implicit membrane region	measure|model	8
1579	Second Slab Thickness	second_slab_thickness	Thickness of a secondary region within the implicit membrane	measure	3
1580	Second Slab Dielectric Constant	second_slab_dielc	Dielectric constant of the secondary implicit membrane region	measure|model	1
1581	Third Slab Thickness	third_slab_thickness	Thickness of a tertiary region within the implicit membrane	measure	2
1582	Third Slab Dielectric Constant	third_slab_dielc	Dielectric constant of the tertiary implicit membrane region	measure|model	1
1583	Ion Concentration	ion_concentration	The molar concentration of salt for the PB calculation	measure	4
1584	Upper Exclusion Radius	upper_exclusion_radius	Upper radius defining the ion-exclusion layer in membrane calculations	measure	2
1585	Lower Exclusion Radius	lower_exclusion_radius	Lower radius defining the ion-exclusion layer in membrane calculations	measure	2
1586	APBS Focussing	do_focussing	Performs a multi-step, iterative grid focusing calculation in APBS	process|method	9
1587	Grid Dimensions	grid_dimensions	The number of grid points along each axis for the PB grid	measure	9
1588	Protein-Protein MM-PBSA	protein_protein	Flag to enable MM-PBSA calculations for a protein-protein complex	method|process	1
1589	Protein 1 Residue Range	protein1_res_range	Defines the residue number range for the first protein partner	identifier	1
1590	Protein 2 Residue Range	protein2_res_range	Defines the residue number range for the second protein partner	identifier	1
1591	Membrane	nonpolar_solv	Sets SASA to zero for residues located inside the membrane	method|identifier	2
1592	extract_WAMMenergies.pl	l	A Perl script to extract final energies from MM-PBSA/GBSA output	software	2
1593	Nonpolar Solvation Energy	NP_SOLV	The nonpolar contribution to the free energy of solvation	measure	2
1594	Polar Solvation Energy	P_SOLV	The polar contribution to the free energy of solvation	measure	7
1595	Total Binding Free Energy	ETOT	The final calculated total binding free energy	measure	2

1596	LIE Calculation Setup	lie_calc	Flag to request the setup of LIE calculations	process	2
1597	LIE Executable	lie_executable	Path to the Perl script that performs LIE calculations	identifier|software	1
1598	First LIE Snapshot	first_lie_snapshot	The starting snapshot for the LIE energy calculation	identifier	3
1599	Last LIE Snapshot	last_lie_snapshot	The ending snapshot for the LIE energy calculation	identifier	3
1600	Offset LIE Snapshots	offset_lie_snapshots	The frequency of snapshots to use in the LIE analysis	identifier	3
1601	Calculate SASA	calc_sasa	Flag to request the calculation of solvent accessible surface area	process	1
1602	extract_LIEenergies.pl	extract_LIEenergies.pl	A Perl script to extract final energies from LIE output	software	2
1603	Soft Core Potential	soft core	A modified potential to avoid singularities during alchemical transformations	model	41
1604	TI Simulation Setup	ti_simulation_setup	Flag to request the setup of files for a TI simulation	process	1
1605	Ligand Name V0	lig_name_v0_struct	Name of the ligand in the initial alchemical state (V0)	identifier	2
1606	Ligand Name V1	lig_name_v1_struct	Name of the ligand in the final alchemical state (V1)	identifier	2
1607	Ligand Alias V0	lig_alias_v0	A three-character alias for the ligand in the V0 state	identifier	2
1608	Ligand Alias V1	lig_alias_v1	A three-character alias for the ligand in the V1 state	identifier	2
1609	Softcore Mask V0	softcore_mask_v0	Atom selection mask for the softcore potential in state V0	identifier|model	1
1610	Softcore Mask V1	softcore_mask_v1	Atom selection mask for the softcore potential in state V1	identifier|model	1
1611	Use PMEMD	use_pmemd	Flag to specify using the PMEMD engine for simulations	identifier|software	3
1612	Prepare Match List	prepare_match_list	Request to generate a list of corresponding non-softcore atoms	process	2
1613	Prepare Inpcrd/Prmtop	prepare_inpcrd_prmtop	Request to generate Amber coordinate and topology files for TI	process	1
1614	TI Equilibration	ti_equil	Flag to request setup of the TI equilibration phase	process	6
1615	TI Equilibration Lambda	ti_equil_lambda	The set of lambda values to be used during TI equilibration	identifier|state	1
1616	TI Production	ti_production	Flag to request setup of the TI production simulation phase	process	9
1617	TI Production Lambda	ti_prod_lambda	The set of lambda values to be used during TI production	identifier|state	1
1618	Total TI Production Time	total_ti_prod_time	The total simulation time requested for each lambda window	measure	1
1619	Convergence Check Method	converge_check_method	Specifies the statistical method for checking TI simulation convergence	method|identifier	1
1620	Convergence Error Limit	converge_error_limit	The numerical threshold used as a termination criterion for convergence	measure	1
1621	TI ddG Calculation	ti_ddG	Request to calculate the final relative binding free energy (ddG)	process	1
1622	dV/dλ	dV/dλ	The derivative of the potential energy with respect to lambda	measure	10
1623	Kruskal's Algorithm	Kruskal	An algorithm to find a minimum spanning tree in a graph	algorithm	3
1624	identify_transformations.pl	l	A script that uses Kruskal's algorithm to find optimal transformations	software	3
1625	TanimotoCombo Score	TanimotoCombo score	A molecular similarity score combining shape and chemical features	measure	1
1626	ROCS	ROCS	Rapid Overlay of Chemical Structures, a shape-based alignment software	software	2
1627	nanosecond	ns	Unit of time commonly used for simulation length	unit	43
1628	Molar	M	Unit of concentration	unit	265
1629	BAR/PBSA	BAR/PBSA	effects	method|model	8
1630	Additive Force Field	additive force fields	Force fields that do not explicitly model electronic polarization	model	8
1631	Ligand Radii Scaling Factor	radiscale	A PBSA keyword to scale the atomic radii of a ligand	identifier|model	11
1632	Protein Radii Scaling Factor	protscale	A PBSA keyword to scale the atomic radii of a protein	identifier|model	8
1633	bar_pbsa.py	bar_pbsa.py	A Python script to automate BAR/PBSA analysis from alchemical simulations	software	8

1634	YAML	YAML	A human-readable data serialization format used for input files	data format	8
1635	Destination Path	dest_path	Location to output processed trajectories and calculation results	identifier	6
1636	Complex Trajectory Paths	complex_paths	Paths to explicit solvent trajectories for the complex system	data source|identifier	2
1637	Ligand Trajectory Paths	ligand_paths	Paths to explicit solvent trajectories for the ligand system	data source|identifier	2
1638	Ion Decharge	ion_decharge	Boolean flag to perform counter-ion decharging for charge neutrality	process|identifier	3
1639	Last Half Frames	last_half_frames	Boolean flag to use only the second half of trajectory frames	process|identifier	2
1640	Frame Subsampling Stride	stride	Step size for subsampling frames from a trajectory	identifier	8
1641	Ligand Residue Name	ligand_res	The residue name of the ligand used to apply radii scaling	identifier	5
1642	Ligand/Complex Selector	ligcom	Option to specify whether 'ligand' or 'complex' trajectories are processed	identifier	2
1643	Delete Trajectory	del_traj	Boolean flag to delete intermediate trajectories to save disk space	process|identifier	2
1644	FE-ToolKit	FE-ToolKit	A library of tools for free energy calculations	software	8
1645	edgembar.OMP	edgembar.OMP	The OpenMP parallelized version of the edgembar program	software	1
1646	Welch's T-test	Welch T-test	A statistical test to determine if two populations have equal means	method	1
1647	p-value tolerance	ptol	The significance level used in the Welch T-test for equilibration detection	measure|identifier	6
1648	Exponential Averaging	exponential averaging	A method to estimate free energy differences, also known as Zwanzig's equation	method|algorithm	10
1649	edgembar-amber2dats.py	edgembar-amber2dats.py	A script to extract DVDL and MBAR data from Amber mdout files	software	7
1650	edgembar-WriteGraphHtml.py	edgembar-WriteGraphHtml.py	A script to perform network analysis and generate an HTML report	software	5
1651	edgembar-bookend2dats.py	edgembar-bookend2dats.py	A script to extract data from MM to QM/MM transformation simulations	software	4
1652	Nonequilibrium Work	nonequilibrium work	Work values from non-equilibrium processes, used in Jarzynski's equality	measure	1
1653	fetkutils-tischedule.py	fetkutils-tischedule.py	A script to optimize the schedule of alchemical states for simulations	software	3
1654	Phase Space Overlap	Phase space overlap (PSO)	A measure of the overlap between distributions of adjacent alchemical states	measure	1
1655	Kullback-Leibler divergence	Kullback-Leibler divergence (KL)	A measure of how one probability distribution diverges from another	measure	1
1656	Small Angle X-ray Scattering	SAXS	An experimental technique to probe the shape and structure of macromolecules	method	14
1657	saxs_rism	saxs_rism	A program to calculate SAXS profiles from 3D-RISM solvent distributions	software	9
1658	saxs_md	saxs_md	A program to calculate SAXS profiles from molecular dynamics trajectories	software	7
1659	Atomic Scattering Factor	f_j(q)	The scattering amplitude of an individual atom as a function of q	measure	1
1660	B-factor	B_j	The Debye-Waller factor, representing atomic displacement/vibration in crystallography	measure	2
1661	Lebedev Quadrature	Lebedev quadrature	A numerical method for integrating functions over the surface of a sphere	algorithm	4
1662	MoFT	MoFT	A suite of programs for analyzing volumetric data	software	15
1663	metatwist	metatwist	An application providing low-level access to MoFT functionalities	software	9
1664	metaFFT	metaFFT	A templated C++ interface to the FFTW library	software	1
1665	OpenDX format	.dx	A file format for storing volumetric data	data format	8
1666	MRC format	.mrc	A binary file format for volumetric data, common in cryo-EM	data format	4
1668	Worm Plot	worm plots	A method to visualize density changes along a curvilinear path	method	2

1669	Twisted/Untwisted Maps	twisted, untwisted maps	Methods to map density onto a plane for helical molecules	method	1
1670	Laplacian of a Gaussian	Laplacian of a Gaussian	A convolution kernel used for feature detection in volumetric data	algorithm	3
1671	Butterworth Filter	Butterworth filter	A type of signal processing filter used for resolution range reduction	algorithm	1
1672	Laplacian Mapping	Laplacian mapping	A method to place water and ions based on the Laplacian of density	method	4
1673	Variational Free Energy Profile	vFEP	A method to compute a free energy surface from biased simulations	method|algorithm	14
1674	Weighted Thermodynamic Perturbation Theory	wTP	A method to predict an unbiased FES from biased sampling	method|algorithm	9
1675	metafile	metafile	The main input file for the ndfes program	data format	33
1676	dumpave file	dumpave	An Amber file containing time-series data of collective variables	data format	63
1677	ndfes.OMP	ndfes.OMP	The OpenMP parallelized version of the ndfes program	software	5
1678	ndfes-PrepareAmberData.py	ndfes-PrepareAmberData.py	A script to prepare metafiles and dumpave files for ndfes	software	17
1679	ndfes-CheckEquil.py	ndfes-CheckEquil.py	A script to detect the equilibrated region of a trajectory	software	13
1680	ndfes-CombineMetafiles.py	ndfes-CombineMetafiles.py	A script to combine multiple metafiles for aggregate analysis	software	6
1681	ndfes-PrintFES.py	ndfes-PrintFES.py	A script to print free energy values from an ndfes checkpoint file	software	3
1682	Reweighting Entropy	reweighting entropy	A measure of the uniformity of MBAR weights within a histogram bin	measure	2
1683	ndfes-AvgFESs.py	ndfes-AvgFESs.py	A script to average multiple free energy surfaces and update errors	software	6
1684	ndfes-path	ndfes-path	A script to analyze and optimize pathways on a free energy surface	software	15
1685	Finite Temperature String Method	finite temperature string method	An algorithm for finding minimum free energy paths on a FES	method|algorithm	5
1686	ndfes-path-prepguess.py	ndfes-path-prepguess.py	A script to create an initial guess for the string method	software	2
1687	ndfes-path-analyzesims.py	ndfes-path-analyzesims.py	A script to prepare string method simulations for analysis	software	3
	Perturbation Theory	gwTP	An extension of the wTP method	method|algorithm	5
	Free Energy Surface	FES	A map of free energy as a function of reaction coordinates	model	68
	ng	ng	The number of grid points in each dimension for the RISM box	identifier	43
	MAP file	MAP file	A file defining ambiguous or partially assigned NMR peaks	data format|data source	8
	Collective Variable Type	cv_type	Keyword specifying the type of reaction coordinate (e.g., DISTANCE, ANGLE).	identifier|model	26
	Atom Type	atom type	A label defining an atom's force field parameters	identifier|model	125
	Surface Offset	b	Offset parameter in the nonpolar solvation energy calculation	measure|model	276
	bb	bb	Input variable for the group transfer free energy of the backbone	identifier|measure	6
	Bond Energy	bond	The energy contribution from valence bonds.	measure	396
	Closure Relation	--closure	An equation to close the Ornstein-Zernike relation in RISM	model|method	6
	CMAP	CMAP	A grid-based energy correction map for protein backbone dihedrals	model|method	32
	Decomposition	dec	Energy decomposition of effective binding free energies	method|process	90
	DFTB Dispersion Correction	dftb_disper	Flag to enable/disable dispersion correction for DFTB2	state	5
	istrng	istrng	The ionic strength of the solution in mM for the PB equation	identifier|measure	22
	LEaP	LEaP	Primary program to create and modify systems for Amber simulations	software	265

	Locally Enhanced Sampling Energy	les	The total energy contributed by the LES copies.	measure	159
	Multidimensional REMD	Multidimensional REMD	REMD simulations involving two or more exchange dimensions (e.g., T and pH).	method|algorithm	8
	offset	offset	A uniform value subtracted from dielectric radii for GB calculations	identifier|measure	53
	Onufriev-Bashford-Case radii	GB^OBC model II	Radii set for a specific Generalized Born model (OBC)	data source|model	0
	Poisson-Boltzmann Energy	pb	The total polar solvation free energy from PB calculations.	measure	168
	REMD Log File	-remlog	Command-line flag to specify the name of the REMD log file.	identifier|software	10
	RISM	RISM	Reference Interaction Site Model of molecular solvation	model|method	266
	gamma	gamma	Phase offset of the dihedral term in degrees.	measure|model	7
	Energy Minimization	energy minimizer	Process of finding a structure's lowest energy conformation	process|method	21
	s"mdiis_restart"	mdiis_restart	Keyword for the MDIIS restart criterion	identifier|measure	12
	mdiis_method	mdiis_method	Keyword to specify the MDIIS implementation	identifier	2
	Gaussian Fluctuation Functional	--gf	Computes the excess chemical potential using the Gaussian fluctuation functional	method|model	2
	PC+/3D-RISM Functional	--pc+	Computes the excess chemical potential using the PC+/3D-RISM functional	method|model	2
	Residue Type	restype	A string property defining the type of a RESIDUE (e.g., protein, solvent)	identifier	7
	Van der Waals Method	vdwmeth	Selects the method for treating van der Waals interactions.	method|model	7
	Ewald Summation Type	ew_type	Selects the type of Ewald summation method.	method|algorithm	10
	Urey-Bradley Energy	angle_ub	The Urey-Bradley contribution to the total energy (CHARMM).	measure	1
	ASM Collective Variable File	CV_file	Path to the file defining the collective variables.	data source	22
	Dimer Method	dimer method	An algorithm for locating transition states on a potential energy surface.	method|algorithm	3
	REMD Type File	-remtype	Command-line flag to specify the name of the REMD type file.	identifier|software	1
	REMD Groupfile	-groupfile	Command-line option specifying the file that defines each replica's simulation.	identifier|software	19
	Number of Replicas	-ng	Command-line option specifying the number of replicas in a simulation.	measure|parameter	39
	REMD Restart Flag	irest=1	Flag to indicate a restart of a simulation, continuing from a previous state.	state|process	15
	Reservoir REMD Type	-rremd	Command-line flag specifying the type of reservoir to use.	identifier|method	1
	Multidimensional REMD File	-remd-file	Command-line flag specifying the multi-dimensional REMD input file.	identifier|software	6